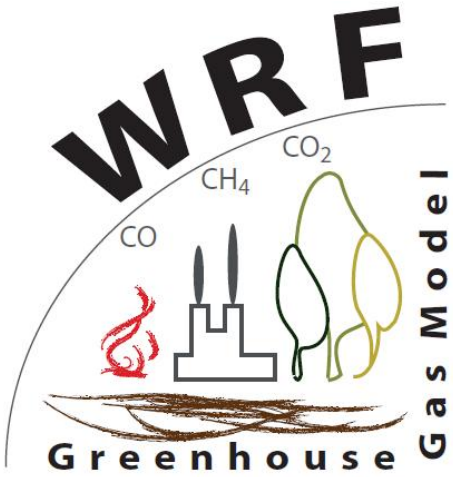
The WRF Greenhouse Gas Model (WRF-GHG)



written by
Veronika Beck[1], Thomas Koch[1], Roberto Kretschmer[1], Julia Marshall[1], Ravan Ahmadov[2,3], Christoph Gerbig[1], Dhanyalekshmi Pillai[1], and Martin Heimann[1]

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[1] Max Planck Institute for Biogeochemistry, Jena, Germany
[2] NOAA Earth System Research Laboratory, Boulder, Colorado, USA
[3] also at: Cooperative Institute for Research in Environmental Sciences, University of Colorado, Boulder, USA

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IMPORTANT NOTE: CODE ACCESS AND COPYING

The WRF-GHG code is copyrighted. This User's Guide is the only documentation provided with this release of WRF-GHG. You may NOT make copies of any part of the code for distribution to any other person or group.

The WRF-GHG source code is distributed for free on request. Please email to Veronika Beck (vbeck@bgc-jena.mpg.de), Thomas Koch (tkoch@bgc-jena.mpg.de), or Christoph Gerbig (cgerbig@bgc-jena.mpg.de) to obtain registration and access information. Afterwards, the source code can be downloaded from the following webpage `http://www.bgc-jena.mpg.de/bgc-systems/index.shtml/` under the button "Download".

If you use WRF-GHG in your research:

- We request that you include the following acknowledgement in the relevant manuscripts: "WRF-GHG is provided by the Max Planck Institute for Biogeochemistry, Germany. MPI assumes no responsibility for the proper use of WRF-GHG by others."
- Please reference WRF-GHG:
  Beck, V., T. Koch, R. Kretschmer, J. Marshall, R. Ahmadov, C. Gerbig, D. Pillai, and M. Heimann, (2011): The WRF Greenhouse Gas Model (WRF-GHG). Technical Report No. 25, Max Planck Institute for Biogeochemistry, Jena, Germany.

If you have made any significant modifications to the code, please mention them in your manuscript.

We are interested to get reports from users about new applications of WRF-GHG, including any problems that come up. If you have questions about the code, appropriate model applications, possible programming errors, etc., please read this entire guide first, and then feel free to contact:

Veronika Beck (vbeck@bgc-jena.mpg.de) or Christoph Gerbig (cgerbig@bgc-jena.mpg.de)

Chapter 1

Overview

In the context of global warming and climate change, carbon dioxide (CO_2) and methane (CH_4), the two most important greenhouse gases, gain more and more attention. In addition to atmospheric observations of greenhouse gases (and additionally, carbon monoxide (CO) used as a tracer for CO_2 and CH_4) and a required thorough understanding of the processes emitting and consuming CO_2 and CH_4, powerful models are indispensable to predict possible impacts of climate change. To achieve this goal, transport simulations of greenhouse gases in the atmosphere at high resolution are essential. Addressing this need, the WRF Greenhouse Gas model was developed to allow for passive tracer transport simulations of CO_2, CH_4, and CO. Several flux models and emission inventories are used for an estimation of the emission and consumption fluxes of CO_2, CH_4, and CO. These flux models are either coupled online, i.e. their code is implemented into the WRF-GHG code or are operated as preprocessors for WRF-GHG to calculate fluxes for the different source and sink processes for CO_2 (autotrophic respiration, photosynthesis, biomass burning, other anthropogenic emissions, termites, ocean sources), CH_4 (wetlands, biomass burning, other anthropogenic emissions, termites, soil uptake) and CO (biomass burning, other anthropogenic emissions).

The main intention of this technical report is to serve as a user guide for WRF-GHG users and developers. The technical report is organized as followed:

The development history of the WRF-GHG code and a detailed description of the WRF-GHG structure is given in Chapter 2. The usage of initial and boundary conditions for the greenhouse gas tracer and the depiction of the different flux models used within WRF-GHG is also found in this chapter.

Chapter 3 focuses on the preprocessors of WRF-GHG. The VPRM-Preprocessor, a biomass burning preprocessor and the Walter wetland model are described in this chapter with the main focus on the installation, configuration and running of the preprocessors.

Namelist settings, compilation, a list of steps how to run WRF-GHG, and a description of the matlab script used to read in CO_2, CH_4, and CO flux fields as well as initial and boundary conditions into the WRF model can be found in Chapter 4.

Everything required to update WRF-GHG to a more recent WRF version (currently WRFV3.2 is used) is described in Appendix A. Appendix B illustrates some results of WRF simulations using WRF-GHG in the Amazon region. In Appendix C, the use of the Model Organizing Software System (MOSS) for automatized simulations of WRF-GHG is explained. The use of open source NCO commands in place of matlab scripts for the manipulation of flux fields and lateral boundary conditions is described in Appendix D.

Chapter 2

The WRF Greenhouse Gas Model (WRF-GHG)

The WRF Greehouse Gas model (WRF-GHG) is an augmentation of the coupled Weather Reasearch and Forecasting model (WRF) to the Vegetation Photosynthesis and Respiration model (VPRM), WRF-VPRM, which is described in detail in Ahmadov et al. [2007] (WRF-VPRM). The main objective of WRF-VPRM is to simulate high resolution passive tracer transport of carbon dioxide (CO_2). WRF-GHG is an extension of WRF-VPRM allowing for passive tracer transport not only for CO_2, but also for methane (CH_4) and carbon monoxide (CO). A further advantage of both WRF-GHG and WRF-VPRM is that initial and boundary conditions can be derived from three-dimensional fields of global simulations of CO_2, CH_4 and CO, e.g. resulting from fluxes optimized by atmospheric inversions on a global scale. CO_2, CH_4 and CO fluxes from different source and sink processes are either calculated "online" (the flux model is implemented in the WRF-GHG code) or "offline" (an external e.g. process-based bottom-up model is used to calculate the fluxes which are then transported inside WRF-GHG).

Chapter 1 first gives a description of WRF-GHG with its newly introduced modules and routines, followed by the set-up for the initial and boundary conditions. Finally, a short illustration of all flux models and datasets used for the calculation of CO_2, CH_4, and CO fluxes concludes this chapter.

2.1 Description of WRF-GHG

2.1.1 Development history of WRF-GHG

The main motivation for developing WRF-GHG was its application to perform regional simulations of CO_2, CH_4, and CO transport in the atmosphere over the Amazon basin during the BARCA (Balanço Atmosférico Regional de Carbona na Amazônia) project. The coupling of the GHG model to the WRF model started with WRF version WRFV3.1.1 and was then upgraded to WRF version V3.2. Meanwhile, WRF-GHG has been tested for Siberia and the Amazon region (both using WRF-GHG based on WRFV3.2 version) and Europe (still as the WRF-VPRM based on WRFV3.0.1 version performing only CO_2 simulations) with different the physics options of the WRF model shown in Table 2.1.

Physics schemes	Options Europe/Siberia
Radiation	rrtm scheme (longwave) Dudhia scheme (shortwave)
Microphysics	WSM 5-class scheme
Cumulus parametrization	Kain-Fritsch (new Eta) scheme
PBL parametrization	YSU or MYJ scheme
Surface layer	Monin-Obukhov scheme
Land surface model	NOAH-LSM

Physics schemes	Options Amazon
Radiation	RRTMG long and short wave
Microphysics	WSM 5-class scheme
Cumulus parametrization	Grell-Devenyi and Grell3
PBL parametrization	MYJ (Eta) TKE scheme
Surface layer	Monin-Obukhov (Janjic Eta) scheme
Land surface model	NOAH-LSM

Table 2.1: Physics options of WRF-GHG used for Europe and Siberia and the Amazon region.

2.1.2 Tracer transport within WRF-GHG

The WRF model (ARW core) uses fully compressible, non-hydrostatic Eulerian equations on an Arakawa C-staggered grid with conservation of mass, momentum, entropy, and scalars [Skamarock et al., 2008]. Tracers are transported online in a passive way, i.e. without any chemical reactions within the framework of the `GHG_TRACER` package with chemistry option 98 (`chem_opt == 98`) in the `namelist.input` file (see Sec. 4.2 for details). Therefore all chemical mechanisms besides vertical mixing are turned off if the tracer transport option is used [Ahmadov et al., 2007]. Online tracer transport implies that transport is performed simultaneously with the meteorological variables at each time step [Ahmadov et al., 2007]. Emissions are added at each time step to the tracer concentration in the lowest model layer. The tracers undergo the advection, boundary layer, and convective mixing as the chemical species. Additionally, from WRFV3.1.1 onwards an option for subgrid convective transport of chemical species has been implemented [Peckham et al., 2009].

In WRF-Chem Version 3.2 a tracer option has already been implemented [Peckham et al., 2009], but here the separate `GHG_TRACER` package is used to allow for online calculation of CO_2 and CH_4 fluxes inside the WRF-Chem model [Grell et al., 2005]. Additionally, other features such as the coupled plumerise mechanism for biomass burning emissions [Grell et al., 2010] are available in the `GHG_TRACER` package which are not available with the standard WRF-Chem tracer option and emissions are handled differently, e.g. no dry deposition.

2.1.3 Description of the code structure of WRF-GHG

Basically, the necessary modifications to the "usual" WRF code for WRF-GHG consist of four additional modules which are added to the WRF-Chem source code and some additional required minor modifications to the WRF-Chem source code itself. The new modules consist of a separate registry file (`registry.ghg`), where all the additional tracer and flux variables used inside WRF-GHG are defined, which is included in the usual WRF-Chem registry (`Registry.EM_CHEM`) and the greenhouse gas module itself (`module_greenhouse_gases.F`) which contains two main parts, the connection of the emissions (fluxes) to the atmospheric concentrations (tracer) and the online calculation of several CO_2 and CH_4 flux fields. Further on, the subroutines for converting fluxes into atmospheric concentrations and adding them to the corresponding tracer variable are located in `module_add_emissions.F`. For biomass burning fluxes and the corresponding tracer, the plumerise model, also part of the standard WRF-Chem [Grell et al., 2010], was modified and adapted to the needs of WRF-GHG and can now be used as an additional option (`module_plumerise_ghg.F`). The subroutine for the greenhouse gas module contains all calls to subroutines for the calculation of online fluxes and the addition of tracer concentrations. It, in turn, is called by the `chem_driver.F` routine in the `<WRFV3/chem>` directory if `chem_opt == 98` is set in the `namelist.input` file.

In the following subsections the four additional modules (`registry.ghg`, `module_add_emissions.F`,`module_greenhouse_gases.F`, and `module_plumerise_ghg.F`) are explained in more detail.

registry.ghg

The `registry.ghg` file is located in the WRF-GHG code in the directory `<WRFV3/Registry>` and included in the main registry of the WRF-Chem model (`Registry.EM_CHEM`). All additional variables for tracers and fluxes used by WRF-GHG, variables needed for the online calculation of fluxes, and all the WRF-GHG-specific namelist options are defined here. For more detailed information on the system of defining variables in the WRF registry see the WRF registry description of Michalakes and Schaffer [2004]. All variables defined in `registry.ghg` are global variables and the empty arrays are created in the `wrfinput` (and additionally also in the `wrfbdy` file) if it is specified in the `namelist.input` file that lateral boundary conditions are requested (for all tracers, see namelist option `have_bcs_chem = .true.` in Sec. 4.2). If it was defined in `registry.ghg`, the variables are also written to the `wrfoutput` file.

All tracers are defined as four-dimensional `chem` arrays in the `registry.ghg` file. The notation is *CO2_1*, ...,*CO2_6* and *CO2_B* for CO_2, *CH4_1*, ...,*CH4_7* and *CH4_B* for CH_4, and *COT_1*, ...,*COT_3* and *COT_B* for CO. The unit of the tracer is $[kg/kg]$. An overview on the assignment of the single tracer variables to different source and sink processes of CO_2, CH_4, and CO is illustrated in Table 2.2.

Additionally, all flux variables representing fluxes of different processes emitting or consuming CO_2, CH_4 and CO are defined in `registry.ghg`. Table 2.3 illustrates a full overview of all fluxes (units in $[kg/m^2s]$) defined in `registry.ghg`. The flux variable

Variable (chem)	Tracer
CO2_1	total atmospheric CO_2 concentration
CO2_2	changes in CO_2 concentration from biogenic activity
CO2_3	changes in CO_2 concentration from anthropogenic emissions
CO2_4	changes in CO_2 concentration from biomass burning
CO2_5	changes in CO_2 concentration from termites
CO2_6	changes in CO_2 concentration from ocean fluxes
CO2_B	atmospheric CO_2 background concentration
CH4_1	total atmospheric CH_4 concentration
CH4_2	changes in CH_4 concentration from wetland emissions
CH4_3	changes in CH_4 concentration from anthropogenic emissions
CH4_4	changes in CH_4 concentration from biomass burning
CH4_5	changes in CH_4 concentration from termite emissions
CH4_6	changes in CH_4 concentration from soil uptake
CH4_7	changes in CH_4 concentration from vegetation
CH4_B	atmospheric CH_4 background concentration
COT_1	total atmospheric CO concentration
COT_2	changes in CO concentration from biomass burning
COT_3	changes in CO concentration from anthropogenic emissions
COT_B	atmospheric CO background concentration

Table 2.2: Overview of all tracer variables defined in the `registry.ghg` file

also defines the time dimension of the external flux which can be either hourly (30 time steps per simulation day) or daily (one time step per day). In case the external fluxes are on different time resolutions, the time dimension of the flux variable can be adjusted in `registry.ghg`. The time resolution of internal calculated fluxes depends on the time step of the model and the output history time step that can be specified in the `namelist.input` file. A detailed description of the online flux calculation and the models coupled online to WRF-GHG follows in Sec. 2.1.3.

Furthermore, all the namelist options that had been established for the WRF-GHG and that are new in the `namelist.input` file are defined here. The last line of the `registry.ghg` file shows how the WRF-GHG is defined: It is defined as chemistry option 98 (`chem_opt=98`) and the package is called `GHG_TRACER`.

module_add_emissions.F

`module_add_emissions.F` contains all subroutines for adding the emissions of CO_2, CH_4, and CO calculated per time step to the corresponding atmospheric concentrations (see Table 2.2). Emissions are usually added to the atmospheric concentrations at the first model layer. All subroutines in this module are called from `module_greenhouse_gases.F`, described in more detail in this section below.

`module_add_emissions.F` consists of the four subroutines `co2_surface_source_add`, `co2_surface_source_ad2`, `add_emis_anthro_ghg`, and `add_emis_burn_ghg`. All these

Variable (`chem_source`)	Flux component	Time Dimension
CO_2		
fl_bio1	ext. biospheric	hourly [30]
fl_oce	ext. ocean	hourly [30]
fl_ant1	ext. anthropogenic	daily [1]
fl_antco2	ext. anthropogenic	hourly [30]
fl_bbco2	ext. biomass burning	daily [1]
bb_co2	3d int. biomass burning	WRF timestep
GEE	int. Gros-Ecosystem-Exchange	WRF timestep
RESP	int. biospheric respiration	WRF timestep
co2_term	int. termite emission	WRF timestep
CH_4		
fl_wet	ext. wetland	hourly [30]
fl_ant4	ext. anthropogenic	daily [1]
fl_antch4	ext. anthropogenic	hourly [30]
fl_bbch4	ext. biomass burning	daily [1]
bb_ch4	3d int. biomass burning	WRF timestep
fl_term	ext. termite emission	daily [1]
fl_soilu	ext. soil uptake	hourly [30]
fl_veg	ext. vegetation	hourly [30]
ch4_emiss	int. wetland	WRF timestep
ch4_term	int. termite emission	WRF timestep
ch4_soil	int. soil uptake	WRF timestep
ch4_veg	int. vegetation	WRF timestep
CO		
fl_ant5	ext. anthropogenic	daily [1]
fl_antco	ext. anthropogenic	hourly [30]
fl_bbco	ext. biomass burning	daily [1]
bb_co	3d int. biomass burning	WRF timestep

Table 2.3: Overview over all flux variables used in the WRF-GHG model that are defined in the `registry.ghg` file. "Ext." implies offline/external calculation of fluxes or use of emission inventories and "int." online calculation of fluxes and internal variables. The time step of the external fluxes can be either daily or hourly. For the internal fluxes the time step of calculation depends on the time step of the WRF model.

subroutines follow the same principle in adding fluxes to atmospheric concentrations. The two-dimensional flux variable `chem_source(i,j)` (for values see Table 2.3) is multiplied by a conversion factor (`conv_rho(i,k,j)`) and added to the first layer of the three-dimensional tracer variable `chem(i,k,j)` (for values see Table 2.2). If the plumerise mechanism is used, biomass burning emissions are added at all vertical layers. The addition of fluxes to the concentrations is illustrated in the following formulas using the variable names of the WRF-GHG source code:

$$chem(i,1,j) = chem\_source(i,j)\left[\frac{kg}{m^2 s}\right] \times conv\_rho(i,1,j)\left[\frac{sm^2}{kg}\right] \qquad (2.1)$$

with

$$conv\_rho(i,1,j) = \frac{1}{rho(i,1,j)[\frac{kg}{m^3}]} \times \frac{dt[s]}{dz8(i,1,j)[m]}. \tag{2.2}$$

Here $rho(i,1,j)$ denotes the air density in the first model layer, dt the time step of the model and $dz8(i,1,j)$ the thickness of the first model layer in [m].

Subroutine `co2_surfac_source_add` is used to add emissions without any specific features using eq. (2.1) to the first model layer. If biomass burning emissions are added into the first model layer, and additionally a diurnal cycle peaking at 18 UTC (14:00 local time) for biomass burning emissions [Prins et al., 1998] is applied (multiplication factor to emissions) subroutine `co2_surfac_source_ad2` needs to be used. If the EDGAR emission inventory is used with an hourly time step containing a diurnal cycle (details in Sec. 2.3.2), but constant for each weekday, the subroutine `add_emis_anthro_ghg` is applied. This multiplies the emissions with a weekly cycle accounting for less traffic on the weekends compared to weekdays [Alonso et al., 2010] before adding them to the first model layer. The multiplication factors are denoted in the following way:

Sun	Mon	Tue	Wed	Thu	Fri	Sat
0.67	1.1	1.1	1.1	1.1	1.1	0.83

For three-dimensional addition of biomass burning emissions in connection with the plumerise mechanism, the subroutine `add_emis_burn_ghg` is deployed. In this case, a loop over all model levels k with their corresponding air density $rho(i,k,j)$ and layer thickness $dz8(i,k,j)$ is conducted in eqs. (2.1, 2.2) in this routine. The addition of the three-dimensional flux fields to the concentration fields also considers the diurnal cycle for biomass burning emissions.

module_greenhouse_gases.F

`module_greenhouse_gases.F` is the main module of WRF-GHG. It contains the main subroutine `greenhouse_gases` which is called from `chem_driver.F`. This subroutine links the emissions to atmospheric concentrations by calling the subroutines in `module_add_emissions.F`. Furthermore the code for all online calculation of fluxes, described in detail in Sec. 2.3, is located here. The different possibilities of offline or online calculation of fluxes (set in `namelist.input`) and the subroutine for adding emissions to atmospheric concentrations are contained in `module_greenhouse_gases.F`. Here, the different possibilities are described briefly.

1. **Anthropogenic emissions except for biomass burning (CO_2, CH_4, CO)**
   In general anthropogenic emissions are taken from an existing external data set and are not calculated online. One can select between inventories at two different time resolutions:

   - Hourly flux inventories
   - Daily flux inventories

For hourly fluxes, the subroutine `add_emis_anthro_ghg` is used to add the emissions to atmospheric concentrations while for the daily fluxes the subroutine `co2_surface_source_add` is used.

2. **Biogenic CO_2 emissions**

   - Online calculated fluxes using the VPRM model [Mahadevan et al., 2008]
   - Externally calculated hourly biogenic CO_2 emissions

   For both, subroutine `co2_surface_source_add` is used to add fluxes to atmospheric concentrations.

3. **CH_4 wetland emissions**

   - Online calculation of CH_4 wetland emissions using the wetland inventory of Kaplan [2002]
   - Offline calculation of CH_4 wetland emissions using the model of Walter et al. [2001a] driven by WRF meteorology

   For both, subroutine `co2_surface_source_add` is used to add fluxes to atmospheric concentrations.

4. **Termite emissions (CO_2, CH_4)**
   Termite emissions are normally calculated online using the model of Sanderson [1996], but an option to use an external dataset exists. Different options for the calculation of termite emissions are possible:

   - Online calculation of CH_4 and CO_2 termite emissions
   - Online calculation of only CH_4 termite emissions
   - Online calculation of only CO_2 termite emissions
   - External dataset for termite emissions for CH_4 and CO_2

   For all cases, subroutine `co2_surface_source_add` is used to add fluxes to atmospheric concentrations.

5. **Biomass burning emissions (CO_2, CH_4, CO)**
   In general the biomass burning emissions are calculated offline by the biomass burning preprocessor [Freitas et al., 2010] (Sec. 2.3.2). The option of using the plumerise mechanism in WRF-GHG exists (see this section below).

   - Plumerise mechanism and a diurnal cycle for the biomass burning emissions are used. Emissions are added in all model layers to atmospheric concentrations (subroutine `add_emis_burn_ghg`)
   - Only biomass burning emissions without plumerise mechanism and diurnal cycle are added to atmospheric concentrations using subroutine `co2_surface_source_add`

- Biomass burning emissions using the diurnal cycle, but no plumerise mechanism (subroutine `co2_surface_source_ad2` used when emissions are added)

6. **Soil uptake (CH_4)**

   - Online calculation of soil uptake fluxes using the model of Ridgwell et al. [1999]
   - External dataset for soil uptake fluxes

   For both, subroutine `co2_surface_source_add` is used to add fluxes to atmospheric concentrations.

7. **CH_4 emissions from vegetation**

   - Online calculation of CH_4 emissions from vegetation as suggested by Keppler et al. [2006]
   - External data set for CH_4 emissions from vegetation

   For both, subroutine `co2_surface_source_add` is used to add fluxes to atmospheric concentrations.

module_plumerise_ghg.F
If the plumerise option is chosen, a one dimensional model calculates the injection height of the biomass burning plume depending on heat fluxes, temperature and wind speed [Freitas et al., 2006, Grell et al., 2010], and determines which fraction of the biomass burning emissions is released at the injection height and at the ground. The plumerise mechanism is part of the official WRF-Chem release, but in WRF-GHG a new module called `module_plumerise_ghg.F` has been established omitting all species usually used with the WRF-Chem model except for CO_2, CH_4, and CO. Basically this plumerise module calls exactly the same subroutines as the plumerise module in the original WRF-Chem code (`module_plumerise1.F`) does.

2.2 Initial and boundary conditions

Simulations are usually performed for a 30 hour run time period with 6 hour spin up for the meteorology from 18 UTC to 24 UTC of the previous day and a 24 hour simulation period of the "actual" simulation day for the tracer transport.

For the meteorology (including Sea Surface Temperature (SST) and soil initialization fields), initial and boundary conditions are taken from the ECMWF operational archive. These data are 6 hourly analysis data of atmospheric model version 1 on 91 hybrid levels with a horizontal resolution of 0.125°. For the Amazon region, the ECMWF soil moisture is replaced by a TRMM-based soil moisture product (GPNR) as the GPNR soil moisture is

considered to be less wet than the ECMWF soil moisture and therefore, more appropriate for this region (S. R. Freitas, M. M. Bela, personal communication).

As initial and boundary conditions for CO_2, CH_4, and CO, three-dimensional fields from global transport models using optimized fluxes from inversions are preferred, as they should describe the distribution of the corresponding greenhouse gas tracer in the atmosphere more realistic than e.g. the standard WRF-Chem profiles. Table 2.4 summarizes the characteristics of the global models used for tracer initialization. In particular, these are the TM3 model used for CO_2 [Rödenbeck et al., 2003], the TM5 model for CH_4 [Bergamaschi et al., 2007, 2009] and the MACC/GEMS re-analysis or near-realtime data for CO (see http://data-portal.ecmwf.int/data/d/gems_reanalysis/levtype=pl/ for re-analysis data and http://data-portal.ecmwf.int/data/d/gems_nrealtime/levtype=pl/ for the near-realtime product). These global fields are then gridded to the WRF grid using the matlab 3d interpolation routine (see Sec. 4.3 for details) and applied as the initial state of the total CO_2, CH_4, and CO concentrations (namely the tracer variables *CO2_1*, *CH4_1* and *COT_1*). For the lateral boundary conditions, the values of the lateral boundary are gradually applied over 5 grid cells in a relaxation zone [Ahmadov et al., 2007], while in WRF-Chem only one layer without relaxation is used.

The initial and boundary conditions for tracers are deployed in the following manner: On the first day of the simulation period of e.g.one month the tracer fields (*CO2_1*, *CH4_1* and *COT_1*) are initialized **once** with the global fields of that day and time, when the tracer transport starts (can be determined by the variable `co2_st_time` in the `namelist.input` file - see Sec. 4.2). For the other time steps of this simulation day only lateral boundary conditions are applied to force the model in the same way as the meteorological boundary conditions do. Hence, for the second day of the simulation period the application of meteorological and tracer initial and boundary conditions differs for the initial conditions, but not for the lateral boundary conditions. The meteorology is initialized with ECMWF fields every day, while the initialization of the tracer variables is taken from the final output of the WRF-GHG simulation at 24 UTC the previous day to ensure continuity. The motivation for re-initializing the meteorology each day is to have a better data constraint of the WRF meteorological fields. Appendix C depicts an example for a Model Organization Software System to perform automatized WRF-GHG simulations with daily re-initialization.

Which tracers are initialized depends on the region for which the simulations are performed. Since the WRF-Chem code does not allow any tracer with negative concentrations, the advected tracer fields "disappear" in case the concentrations become negative. This can happen even though the positive definite advection scheme is used. It is avoided by initializing all tracer with the global fields or an offset (and also force them with lateral boundary conditions) and later subtract the offset or the global background which can be transported inside the WRF-GHG model as a separate tracer for this purpose. This problem was first discovered for simulations in the Amazon region, and therefore all tracers should be initialized with background or offset for this region. It might also occur in other regions where local sources are very strong and therefore, producing strong gradients.

Model	Horizontal resolution	No. of vertical levels	Time interval
TM3	$\sim 4° \times 5°$	19	6 hourly
TM5	$6° \times 4°$	25	daily
MACC	$1.125° \times 1.125°$	60	6 hourly

Table 2.4: Main characteristics of the global models used as initial and lateral boundary conditions in WRF-GHG.

Thus, for Europe or other mid-latitude regions only the tracer for the total CO_2, CH_4 and CO concentration (*CO2_1*,*CH4_1* and *COT_1*) and the tracer for the background concentration of CO_2, CH_4 and CO (*CO2_B*,*CH4_B* and *COT_B*) are initialized with global fields and are forced on the lateral boundaries. Special care has to be taken for the tracers *CO2_2* and *CH4_6*–concentrations from VPRM and soil uptake fluxes. Because their corresponding fluxes can become negative, if they are not initialized with the global fields they have to be set to a constant offset (0.0002 for *CO2_2* and 10^{-7} for *CH4_6*, respectively) to avoid problems in WRF-GHG with negative concentration values. For the analysis of the output fields, this offset is subtracted.

2.3 CO_2, CH_4, and CO fluxes in WRF-GHG

In this section a short description of the different models and emission inventories used for the calculation of CO_2, CH_4 and CO fluxes, that are then transported inside WRF-GHG, is given. For the flux models that are implemented inside the WRF-GHG code, the description provides more in detail on the implementation of these models and how they had been adapted to match the WRF requirements. An overview of the external data sets that are used within WRF-GHG is found in the second part of this section.

2.3.1 Online calculated fluxes

Fluxes calculated online in WRF-GHG are mainly biogenic emissions of the trace gases such as the biogenic CO_2 fluxes using the VPRM model, CH_4 fluxes from wetlands using the wetland inventory from Kaplan [2002], termite emissions of CO_2 and CH_4, soil uptake of CH_4 and CH_4 emissions from vegetation. All subroutines for the online calculation of fluxes are located in `module_greenhouse_gases.F` inside the WRF-GHG code.

Biospheric CO_2 fluxes - the VPRM model

The Vegetation Photosythesis and Respiration Model (VPRM) is a diagnostic model that calculates hourly Net Ecosystem Exchange (NEE) based on Moderate Resolution Imaging Spectroradiometer (MODIS) satellite estimates of the Land Surface Water Index (LSWI) and Enhanced Vegetation Index (EVI), short wave radiation and surface temperature. A detailed description of the VPRM model is found in Mahadevan et al. [2008].

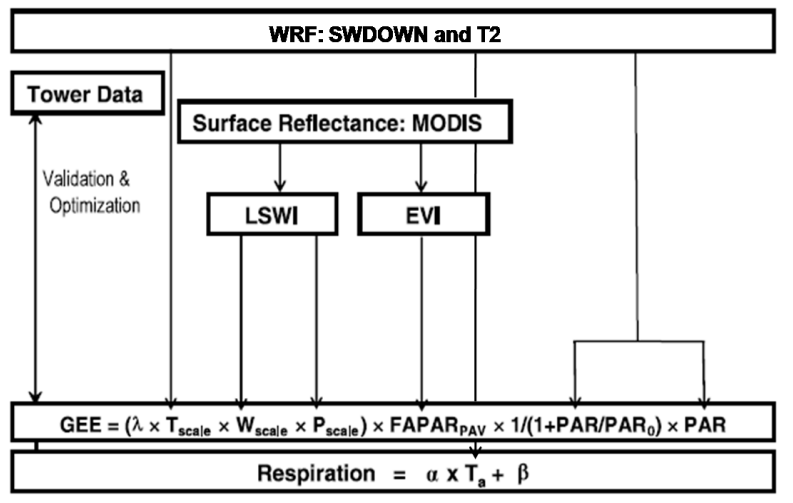

WRF: SWDOWN and T2
Tower Data
Surface Reflectance: MODIS
Validation & Optimization
LSWI
EVI
GEE = (λ × T_scale × W_scale × P_scale) × FAPAR_PAV × 1/(1+PAR/PAR_0) × PAR
Respiration = α x T_a + β

Figure 2.1: Schematic structure of the VPRM model calculating GEE and Respiration based on satellite data and input variables from WRF. The VPRM parameters themselves (λ, PAR_0, α, β) are validated against Eddy-flux tower data (adapted from Mahadevan et al. [2008]).

Fig. 2.1 illustrates the basic structure of the VPRM model. LSWI and EVI from MODIS satellite data are included in the variables P_{scale} to account for the effects of leaf age on photosynthesis and W_{scale} to account for the effects of water stress. The equation to calculate the Gross Ecosystem Exchange (GEE) in the VPRM model is written as:

$$GEE = \lambda \times T_{scale} \times P_{scale} \times W_{scale} \times EVI \times \frac{1}{1 + \frac{PAR}{PAR_0}} \times PAR \tag{2.3}$$

where λ is a factor for the maximum quantum yield and PAR_0 is the half-saturation value of the photosynthetically active radiation (PAR). Both values are adjustable and determined by analysis of data from eddy covariance towers. The parameter T_{scale} represents the temperature dependence of the photosynthesis, depending on minimum, maximum and optimal temperature (T_{min}, T_{max} and T_{opt}) for the photosynthesis process [Raich et al., 1991]. The VPRM model uses 8 different vegetation classes. For each vegetation class, the values of T_{min}, T_{max} and T_{opt} are defined in the VPRM subroutine in `module_greenhouse_gases.F` as given in Table 2.5.

Vegetation class	T_{min} [°C]	T_{max} [°C]	T_{opt} [°C]
Evergreen forest	0	40	20
Deciduous forest	0	40	20
Mixed forest	0	40	20
Shrubland	2	40	20
Savanna	2	40	20
Cropland	5	40	22
Grassland	2	40	18
Others	0	40	0

Table 2.5: T_{min}, T_{max} and T_{opt} values for the photosynthesis process as defined in WRF-GHG.

The short wave incoming radiation (SWDOWN) of the WRF model is used as a proxy for the photosynthetically active radiation (PAR).
The respiration process is parameterized as a function of temperature:

$$Resp = \alpha \times T_a + \beta \tag{2.4}$$

with adjustable parameters α and β that are determined by comparison to the data from eddy covariance measurements. For the temperature T_a [°C], the 2m temperature from WRF is used. The Net Ecosystem Exchange (NEE) is calculated as the sum of GEE and respiration:

$$NEE = \lambda \times T_{scale} \times P_{scale} \times W_{scale} \times EVI \times \frac{1}{1 + \frac{PAR}{PAR_0}} \times PAR + \alpha \times T_a + \beta \tag{2.5}$$

In WRF-GHG the VPRM parameters are read in from an external `*.txt` file (e.g. `VPRM_param_CERES2005_local.txt` for Europe) stored in the `<WRFV3/run/CO2_input>` directory. The name of this file can be specified in the `namelist.input` file. GEE and respiration (RESP) are defined as global variables and are found as hourly fluxes in the `wrfoutput` file.

CH_4 fluxes from wetlands (I) - the Kaplan inventory

The wetland inventory developed by Kaplan [Kaplan, 2002, Drevet, 2008] is based on a diagnostic approach to determine CH_4 emissions from wetlands as a percentage of the heterotrophic respiration [Christensen et al., 1996]. The main drivers for calculating the

carbon decomposition rate k_r, which is a measure of the amount of carbon decomposed in a certain time frame that further determines the amount of heterotrophic respiration, are soil moisture availability and soil temperature, which are both taken from the WRF model. In addition, an external carbon pool (CPOOL - from the LPJ model [Sitch et al., 2003]) representing the substrate availability and a wetland map (WETMAP - Kaplan potential wetland map [Kaplan, 2002, Bergamaschi et al., 2007]) are necessary external input fields for the determination of the wetland fraction per grid cell. The calculation of the carbon decomposition rate k_r follows Sitch et al. [2003] depending on a soil moisture factor f_{SM} and a temperature dependence $g(T)$:

$$k_r = \frac{\frac{1}{\tau_0} \cdot g(T) \cdot f_{SM}}{12 \cdot 24 \cdot 30}. \tag{2.6}$$

with $\tau_0 = 2.86a$ as a factor accounting for the turnover time of the fast carbon pool. The soil moisture factor f_{SM} is expressed as:

$$f_{SM} = 0.25 + 0.75 \frac{sm}{sm_{sat}} \tag{2.7}$$

with sm indicating the mean value of the first two soil moisture (SMOIS) layers of the WRF model and sm_{sat} the saturation value of the soil moisture depending on the soil type. This value was obtained from the `SOILPARM.TBL` in the `<WRFV3/run>` directory and then linked to the soil types of the WRF model in the subroutine of the Kaplan wetland inventory. Additionally, k_r depends on the soil temperature (first layer of the soil temperature (TSLB) is taken) in the following way:

$$g(T) = \exp\left(308.56 \cdot \left(\frac{1}{56.02} - \frac{1}{T + 46.01}\right)\right). \tag{2.8}$$

In the WRF model, the soil temperature is only defined for land grid points. But as wetland emissions also occur close to rivers and lakes, a wetland fraction might exist for a grid point which is defined as water (and not as land in the WRF land-sea mask). For those grid points, the soil temperature in WRF is not defined and the value of the skin temperature (TSK) is used instead.

The amount of decomposed carbon per second is determined based on exponential decay. Heterotrophic respiration is assumed to be 70% of the decomposed carbon in the fast carbon pool calculated with the help of k_r. Using different scaling factors depending on the type of the wetland ($E_f = 0.05$ for peatland and $M_s = 0.19$ floodplain [Drevet, 2008]), the amount of CH_4 emissions is calculated from the derived heterotrophic respiration. If peatland and floodplain coexist (e.g. for global applications), a weighting factor P_l is introduced that depends on the mean annual temperature T_a (obtained from an external dataset) [Drevet, 2008]:

$$P_l = \exp\left(\frac{T_a - 303.0}{8}\right). \tag{2.9}$$

The global carbon pool from the LPJ model and the Kaplan potential wetland map are read into the `wrfinput` file via a matlab script (Sec. 4.3). The calculation itself is performed online and the calculated CH_4 wetland fluxes are stored in the variable *CH4_EMISS* in the `wrfoutput` file.

Termite CO_2 and CH_4 fluxes

The calculation of CO_2 and CH_4 emissions from termites follows the description of a global data base for termite emissions as described in Sanderson [1996]. The trace gas flux emitted by termites per m^2 is calculated as the product of biomass of termites [g/m^2] and the flux of trace gas emitted from those termites [g gas/g termite and hour]. The amount of termites per gram of biomass depends on the vegetation type and was determined by measurements in the same way as the trace gas emissions per amount of termites [Sanderson, 1996]. In the database daily constant values of termite emissions are assumed even though there was evidence for a diurnal variation of termite emissions [Sanderson, 1996]. Furthermore, Sanderson [1996] distinguishes between termite emissions in the old world (Europe, Asia, Africa) and the new world (America, Australia). Table 2.6 illustrates the mapping of the vegetation types used by Sanderson [1996] to the WRF vegetation types, which are the basis for calculating the biomass per grid cell and determining the termite flux values.

Soil uptake CH_4 fluxes

The soil uptake model developed by Ridgwell et al. [1999] is a process-based model to calculate the consumption of atmospheric CH_4 by soils. The CH_4 flux into the soil is calculated by the following formula:

$$J_{CH4} = \frac{C_{0CH4} D_{CH4}}{z_d}\left(1 - \frac{D_{CH4}}{D_{CH4} + k_d z_d}\right) \times F \tag{2.10}$$

with J_{CH4} indicating the flux of CH_4 into the soil, D_{CH4} the diffusivity of the topsoil, C_{0CH4} the atmospheric CH_4 concentration (here the total CH_4 concentration of the WRF-GHG variable *CH4_1* is taken), z_d the soil depth in cm, k_d the first-order oxidation rate, and F a factor 616.9 mg $ppmv^{-1}$ cm^{-1} CH_4 to account for unit conversions. This equation (based on Fick's law with some modifications to account for changes in microbial oxidation activity) implies that the main part of the oxidation takes place at a soil depth of z_d =6 cm. The soil diffusivity D_{CH4} is described by:

No.	WRF vegetation type (IVGTYP)	Vegetation type after Sanderson [1996]
1	Urban and built up land	-
2	Dry cropland and pasture	Farmland, settlement
3	Irrigated cropland, pasture	Farmland, settlement
4	Mixed dryland, irrigated cropland, pasture	Patchy wood, crop/grass
5	Cropland/grassland mosaic	Patchy wood, crop/grass
6	Cropland/woodland mosaic	Patchy wood, crop/grass
7	Grassland	Temperate grassland
8	Shrubland	Tree, shrub
9	Mixed grassland/shrubland	Tree, shrub
10	Savanna	Savannyh/grassland - arid
11	Deciduous broadleaf forest	Temperate forest
12	Deciduous needleleaf forest	Temperate forest
13	Evergreen broadleaf forest	Tropical rainforest, raingreen forest, tropical montane forest
14	Evergreen needleleaf forest	Raingreen forest
15	Mixed forest	Temperate forest
16	Water bodies	-
17	Herbaceous wetland	-
18	Wooden wetland	-
19	Barren/sparsely vegetated	dry highland/shrub
20	Herbaceous tundra	-
21	Wooded tundra	-
22	Mixed tundra	-
23	Bare ground tundra	-
24	Snow or ice	-

Table 2.6: Illustration on how vegetation types defined by Sanderson [1996] are assigned to WRF vegetation types for the quantification of termite fluxes.

$$D_{CH4} = G_{soil} \times G_T \times D_{0CH4} \tag{2.11}$$

where D_{0CH4} is the diffusivity of CH_4 in free air and G_{soil} and G_T are factors that account for the effects of the soil structure and soil temperature, respectively. The variable G_{soil} is expressed as:

$$G_{soil} = \Phi^{\frac{4}{3}} \left(\frac{\epsilon}{\Phi}\right)^{1.5+\frac{3}{b}}. \tag{2.12}$$

Φ indicates the total pore volume and ϵ the air-filled porosity which are both taken according to the soil type (ISLTYP) from the WRF parameter soil table `SOILPARM.TBL`. In addition, the sand content (I_{sand}) of each soil type is taken from this table. The clay content (I_{clay}) of each soil type is determined after Cosby et al. [1984]. From these values, the parameter b can be calculated:

$$b = -3.140 - 0.00222 \cdot I_{clay}^2 - 3.484 \cdot 10^{-5} \cdot I_{sand}^2 \cdot I_{clay}. \tag{2.13}$$

The dependence on the soil temperature is expressed with the following equation:

$$G(T) = 1.0 + 0.0055 \cdot T \tag{2.14}$$

with the soil temperature in °C being the WRF soil temperature of the second soil layer. The CH_4 oxidation rate k_d consists of factors for three different influences: the cultivation influence (r_N), the temperature influence (r_T) and the soil moisture influence (r_{SM}) and is defined as following:

$$k_d = r_N \times r_T \times r_{SM} \times k_0 \tag{2.15}$$

with k_0 being the base oxidation rate, constant for uncultivated soil at 0°C. As soil uptake is reduced due to agricultural activity and use of fertilizers, the cultivation factor r_N takes into account the cultivation activity of the vegetation type:

$$r_N = 1.0 - (0.75 \times I_{cult}) \tag{2.16}$$

where I_{cult} is a measure of the cultivation activity of the vegetation type. Using the WRF vegetation types (cf. Table 2.6), I_{cult} is set to 1 for vegetation types ≤ 5, to 0.5 for vegetation type = 6 and to 0 for all other vegetation types. The dependence of the oxidation rate on temperature is based on a Q_{10} approach:

$$r_T = \exp\left(0.0693 \cdot T - 8.56 \cdot 10^{-7} \cdot T^4\right) \tag{2.17}$$

for temperature >0°C and a value of 0 for temperatures <0°C. The soil moisture effect on the oxidation activity is set to 1.0 if the sum of precipitation and soil moisture divided by potential evaporation is greater than 1.0 or the sum of precipitation and soil moisture divided by potential evaporation itself in case the calculated factor is smaller than 1.0.

The following variables from the WRF model are used to drive the soil uptake model: Soil moisture (SMOIS), soil type (ISLTYP) and soil parameters (`SOILPARM.TBL`), total CH_4 atmospheric concentration (CH4_1), precipitation (RAINC + RAINNC), potential evaporation (POTEVP), landuse (LANDUSE), soil temperature (TSLB) and the wetland map (WETMAP) to exclude soil uptake for grid cells that are mainly covered by wetland area.

CH_4 flux from vegetation

In 2006 Keppler et al. [2006] published their findings on CH_4 emissions from plants. The discussion about CH_4 emission from vegetation is still controversial [Ferretti et al., 2007, Dueck et al., 2007, Beerling et al., 2008, Houweling et al., 2006]. Thus in WRF-GHG a CH_4 vegetation source has been implemented for hypothesis testing. The emissions for day and night ($emiss\_day = 374 \cdot 10^{-9}\ \frac{kgCH_4}{kgbiomass/hr}$, $emiss\_night = 119 \cdot 10^{-9}\ \frac{kgCH_4}{kgbiomass/hr}$)

are scaled with the values of GEE and RESP from the online calculation of the VPRM model:

$$Vegetation_{CH4} = -2.0 \cdot emiss\_day \cdot GEE \tag{2.18}$$

for daytime emissions (i.e. when the incoming shortwave radiation (SWDOWN) exceeds a threshold value of 50.0) and nighttime emissions of

$$Vegetation_{CH4} = 2.0 \cdot emiss\_night \cdot RESP \tag{2.19}$$

The factor of two accounts for the conversion of GEE and RESP to plant biomass. For agricultural WRF vegetation types (1-6 see Table 2.6), the emissions are assumed to be 88.5% of the emissions for vegetation types with no agricultural activity [Keppler et al., 2006].

2.3.2 External flux data sets

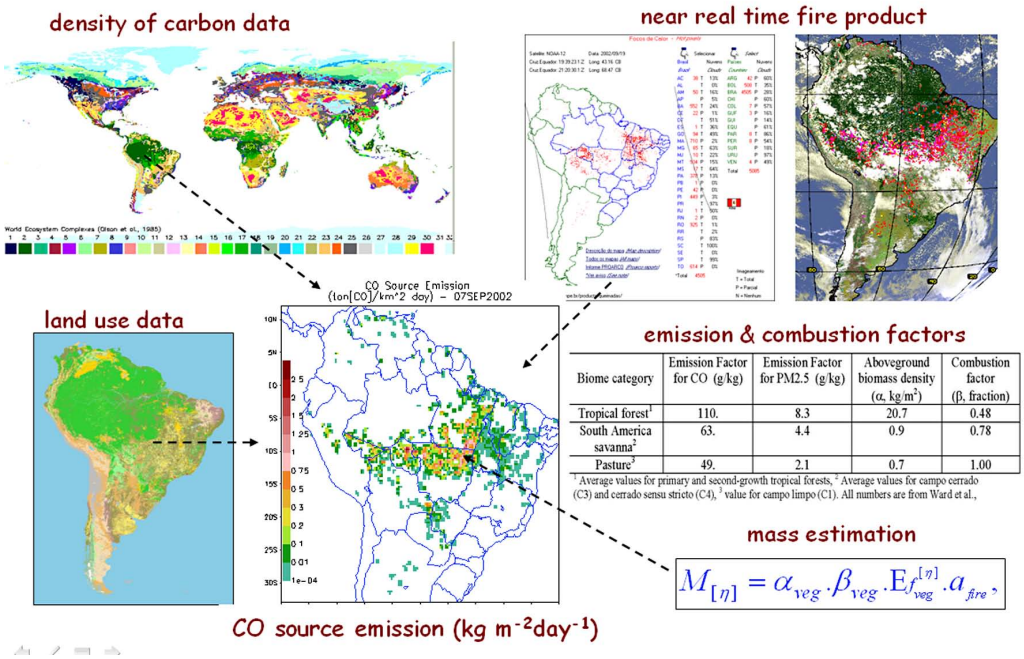
External data sets are read into the `wrfinput` file and are transported within WRF-GHG. All external data have to be gridded to the WRF grid, e.g. by using NCL tools (function rgrid2rcm) or an R script, before they are read into the `wrfinput` file via a matlab script (see Sec. 4.3). For anthropogenic emissions, the inventories of EDGAR and IER have been used so far. Biomass burning emissions are calculated with the biomass burning preprocessor *Prep_chem_sources* (more details in Sec. 3.2) and external wetland fluxes are calculated by the Walter wetland model driven by WRF meteorology. Ocean fluxes of CO_2 can also be transported inside WRF-GHG.

Biomass burning emissions for CO_2, CH_4 and CO

Biomass burning emissions are calculated as daily emissions based on satellite fire spots by a WRF-Chem preprocessor (*Prep_chem_sources*) developed by Karla Longo and Saulo Freitas. A complete description of this preprocessor can be found in Freitas et al. [2006], Longo et al. [2007], Freitas et al. [2010]. Here, a brief description of the theory how the biomass burning fluxes are calculated is given, while Sec. 3.2 deals more with the technical issues of running the *Prep_chem_sources* preprocessor.

The satellite fire database uses three different satellites:

- GOES WF_ABBA (Geostationary Operational Environmental Satellite - Wildfire Automated Biomass Burning Algorithm)


density of carbon data
near real time fire product
CO Source Emission
(ton[CO]/km^2 day) - 07SEP2002
land use data
emission & combustion factors
mass estimation
$M_{[\eta]} = \alpha_{veg} . \beta_{veg} . \mathrm{E}f_{veg}^{[\eta]} . a_{fire}$
CO source emission (kg m-2day-1)

Biome category	Emission Factor for CO (g/kg)	Emission Factor for PM2.5 (g/kg)	Aboveground biomass density (α, kg/m^2)	Combustion factor (β, fraction)
Tropical forest[1]	110.	8.3	20.7	0.48
South America savanna[2]	63.	4.4	0.9	0.78
Pasture[3]	49.	2.1	0.7	1.00

[1] Average values for primary and second-growth tropical forests, [2] Average values for campo cerrado (C3) and cerrado sensu stricto (C4), [3] value for campo limpo (C1). All numbers are from Ward et al.,

Figure 2.2: Schematic structure of all input parameters for the biomass burning preprocessor (from Longo et al. [2007]).

- Brazilian National Institute for Space Research fire product based on AVHRR (Advanced Very High Resolution Radiometer) onboard the NOAA polar orbiting satellite series
- MODIS (Moderate Resolution Imaging Spectroradiameter) fire product

A filter is applied to avoid double counting of fire pixels. For each fire pixel that is detected, the mass of emitted tracers is calculated using the following equation:

$$M^{[\eta]} = \alpha_{veg} \cdot \beta_{veg} \cdot EF_{veg}^{[\eta]} \cdot a_{fire} \tag{2.20}$$

with $M^{[\eta]}$ being the emitted mass of the tracer η. α_{veg} describes the above ground biomass available for burning, β_{veg} the combustion factor after Ward et al. [1992], $EF_{veg}^{[\eta]}$ the emission factor for each species η after Andreae and Merlet [2001] and a_{fire} the area of the fire. The GOES WF_ABBA satellite retrievals also give an estimate of the burnt area of each fire. In case there are no estimates of the firesize available from the satellite observations, a mean fire size of 0.14 km^2 for the GOES WF_ABBA detected fires and 0.22 km^2 for the MODIS and AVHRR detected fires is assumed [Longo et al., 2007].

The fire detection maps are then merged with 1 km landuse maps and the carbon live vegetation dataset (Fig. 2.2) and multiplied by the emission factors of Andreae and Merlet [2001] and the combustion factor for the different vegetation types. The output emissions

are in units of [kg/m^2 day]. These emissions can be combined with a diurnal cycle for biomass burning [Prins et al., 1998] in WRF-GHG as described in Sec. 2.1.3. Additional variables for using the plumerise mechanism in WRF-GHG (Sec. 2.1.3), such as the mean firesize, etc. are also available as output from this preprocessor.

Anthropogenic emissions for CO_2, CH_4 and CO

For anthropogenic emissions (except for biomass burning emissions), WRF-GHG has been tested with EDGAR (Amazon) and IER (Europe) emission inventories.

The EDGAR V4.1 emission inventory (available online via http://edgar.jrc.ec.europa.eu) is on a $0.1^\circ \times 0.1^\circ$ resolution and globally available for greenhouse gases such as CO_2 and CH_4 and other trace gases, e.g.CO, on a yearly basis up to 2005. All IPCC categories can be downloaded from the webpage and have to be summed up to get the final emissions. The emissions are gridded on the WRF grid using the biomass burning preprocessor *Prep_chem_sources* (see previous Section and Sec. 3.2). Additionally, an update for major cities in South America has been added to the preprocessor including a scaling of the emissions with the number of vehicles in larger cities and a diurnal cycle for the EDGAR emissions depending on the traffic flow. This work was done by Alonso et al. [2010]. A weekly cycle for the EDGAR dataset can be applied by using the subroutine `add_emis_anthro_ghg` for adding the emissions to the concentrations as described in Sec. 2.1.3.

For CO_2 fossil fuel emissions over Europe, the IER (Institute of Economics and the Rational Use of Energy, University of Stuttgart) dataset on 10 km horizontal resolution can be used (available on request via http://carboeurope.ier.uni-stuttgart.de). This dataset contains hourly emissions of greenhouse gases for the year 2000. To apply the dataset to other years, a shift in the weekdays was taken into account [Ahmadov et al., 2007, Pillai et al., 2010]. The code for preprocessing the IER data can be requested via email from Roberto Kretschmer (rkretsch@bgc-jena.mpg.de).

CH_4 fluxes from wetlands (II) - the Walter model

The Walter wetland model [Walter et al., 1996, Walter and Heimann, 2000, Walter et al., 2001a,b] is a process-based model to calculate CH_4 emissions from wetlands. The most important factors influencing CH_4 wetland emissions are taken into account:

- Position of the water table to separate between anaerobic production of CH_4 and aerobic conditions for oxidation of CH_4
- Soil temperature to control the rate of methanogenesis
- Transport of CH_4 to the atmosphere through the different mechanisms of plant mediated transport, ebullition and diffusion

The one-dimensional model itself consists of 170 layers with a thickness of 1 cm and the change of CH_4 concentration (C_{CH4}) with time at each soil layer (z) is expressed through the following equation:

$$\frac{\partial}{\partial t}C_{CH4}(t,z) = -\frac{\partial}{\partial z}F_{diff}(t,z) + Q_{ebull}(t,z) + Q_{plant}(t,z) + R_{prod}(t,z) + R_{oxid}(t,z) \tag{2.21}$$

where the main terms are defined as follows:

- *CH_4 diffusion flux F_{diff}* described through the equation below is based on Fick's law and depends the diffusion coefficient of CH_4 (D_{CH4}) and the CH_4 concentration gradient at depth z.

$$F_{diff}(t,z) = -D_{CH4}(z)\frac{\partial}{\partial z}C_{CH4}(t,z) \tag{2.22}$$

- *CH_4 ebullition flux rate Q_{ebull}* is > 0 if the CH_4 concentration in a soil layer exceeds a certain threshold value C_{thresh}. Then 70% of the CH_4 released in bubbles is transported to the layer at the height of the water table and the other 30% is trapped in the upper part of the water saturated layers.

- *The plant-mediated transport rate (Q_{plant})* tells how much CH_4 is transported to the atmosphere through plants and depends on the efficiency of plant-mediated transport (IT-VEG), the growing state of the plants, the vertical distribution of the roots in the soil, and the CH_4 concentration in the corresponding soil layer.

- *The CH_4 production rate (R_{prod})* depends on the substrate availability with depth, the amount of substrate itself (NPP), and the soil temperature.

- *The CH_4 oxidation rate (R_{oxid})* follows the Michaelis-Menten kinetics with a Q_{10} soil temperature dependence.

The position of the water table as separator between the soil layers below the water table where anaerobic microbial production of CH_4 takes place and the soil layers above the water table is calculated from an adjoint hydrological model where the soil of each grid point is considered as a bucket of 1.7 m depth (a complete description of the hydrological model is found in Walter et al. [2001a]). The aim of the hydrological model is to calculate fluctuations of the water table as a functions of climatological parameters (precipitation, 2 m air temperature, surface solar radiation). Evapotranspiration, lateral inflow and runoff are calculated within the hydrological model to determine the position of the water table which serves as an input for the Walter wetland model.

The Walter wetland model is described in detail in Walter et al. [1996], Walter and Heimann [2000], but Fig. 2.3 gives a quick overview over the structure of the model. The

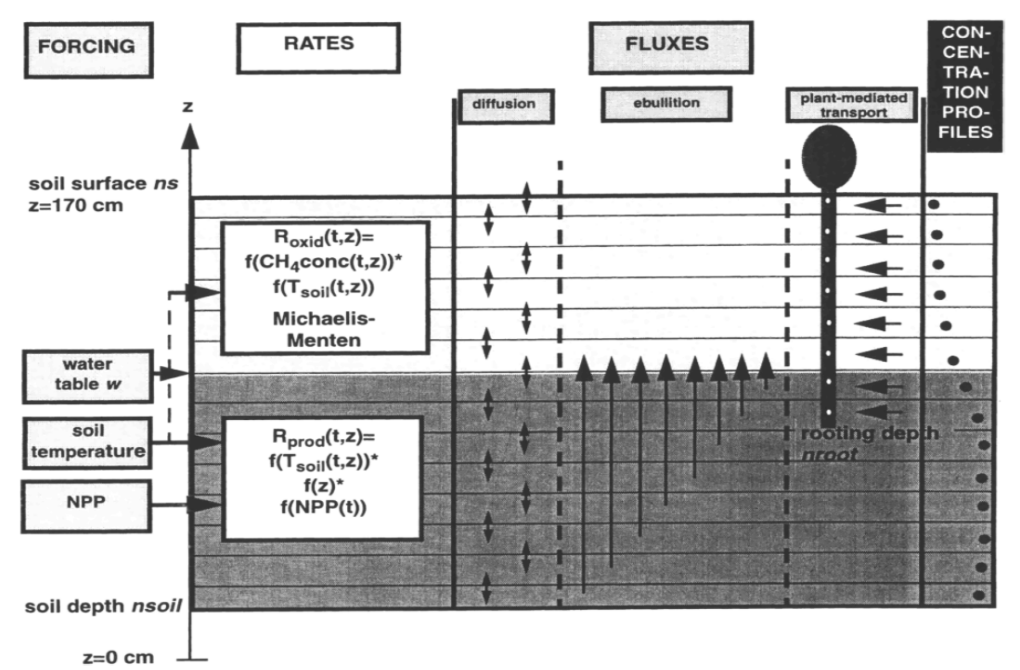


Figure 2.3: Schematic representation illustrating the structure of the Walter wetland model with the position of the water table, soil temperature, and NPP as input of the model. The CH_4 production and oxidation rates that are calculated at each soil layer and the three different processes (diffusion, ebullition and plant-mediated transport) are responsible for the transport of the CH_4 to the atmosphere (from Walter and Heimann [2000]).

emissions are calculated at each wetland grid point separately and then multiplied with the fractional coverage of wetland area in that grid cell. This information is obtained from a wetland map. In this case we used the Kaplan potential wetland map that was already described in Sec. 2.3.1.

Up to now an online calculation of CH_4 wetland fluxes using the Walter model is not implemented, but the offline version of the model is driven by WRF meteorological output fields (Precipitation (RAINC+RAINNC), soil temperature (TSLB), radiation and heat fluxes (SWDOWN,GLW) and surface temperature (T2)). Additionally, soil and vegetation properties such as root and soil depth used in the Walter wetland model [Walter et al., 2001a] have been derived from the WRF vegetation and soil types as shown in Table 2.7.

Other necessary input fields besides the wetland map are daily net primary productivity (NPP) values, mean annual soil temperature, and an elevation map. These maps (except for the wetland map) are gridded from the Walter et al. [2001a] version to the WRF model grid and missing values are filled in as described in Sec. 3.3.

WRF veg. type	Walter veg. type	IT-VEG	nroot [cm]	nsoil [cm]	ibare [%]	inppm [$\frac{gC}{m^2yr}$]	inppt [$\frac{gC}{m^2yr}$]	rpv
1	0	0.0	0	0	0	0	0	0
2	0	0.0	0	0	0	0	0	0
3	0	0.0	0	0	0	0	0	0
4	0	0.0	0	0	0	0	0	0
5	1/3 (50%)	5.0	39.23	79	20	120	701	0.34
6	1/3 (50%)	0.5	64.41	129	5	110	1141	0.29
7	4	15.0	81.07	162	5	100	829	0.19
8	2	0.0	62.86	126	20	120	701	0.34
9	2/4 (50%)	7.5	71.96	144	9	124	931	0.22
10	3	10.0	39.23	79	5	100	829	0.19
11	1	1.0	66.56	129	5	110	1141	0.29
12	1	1.0	98.95	129	5	110	1141	0.29
13	1	1.0	57.88	129	5	110	1141	0.29
14	1	1.0	59.43	129	5	110	1141	0.29
15	1	1.0	64.41	126	5	110	1141	0.29
16	6	15.0	39.23	79	5	100	829	0.19
17	6	15.0	39.23	79	5	100	829	0.19
18	1/6 (50%)	7.0	51.82	104	9	124	931	0.22
19	2	0.0	62.86	126	20	120	701	0.34
20	5	10.0	25.60	51	5	100	829	0.19
21	1/5 (50%)	5.0	45.00	89	20	120	701	0.34
22	1/5 (50%)	5.0	45.00	89	20	120	701	0.34
23	5	10.0	25.60	51	5	100	829	0.19
24	0	0.0	0	0	0	0	0	0

Table 2.7: Parameter table to match the vegetation types defined by Walter et al. [2001a] and the WRF vegetation types and assigned parameters for efficiency of plant-mediated transport (IT-VEG = 0 no plant mediated transport =15 maximum efficiency for plant mediated transport), rooting depth (*nroot*), soil depth (*nsoil*), fraction of bare soil (*ibare*), maximum monthly NPP (*inppm*), total annual NPP (*inppt*) and relative pore space of coarse pores (*rpv*, between 0 and 1). Most of the parameter values are derived from the parameter table in Walter et al. [2001a]. The Walter vegetation types with a 50% indication are the average of two different vegetation types. The rooting depth was calculated after the corresponding formula in Walter et al. [2001a].

Ocean CO_2 fluxes

Ocean CO_2 can be obtained on a $4^\circ \times 5^\circ$ grid from Takahashi et al. [2009].

Chapter 3

WRF-GHG Preprocessors

For preprocessing the flux fields or other parameter fields that are necessary for the online calculation of fluxes in WRF-GHG, two main preprocessors are used for WRF-GHG, the VPRM-Preprocessor, to obtain EVI, LSWI and vegetation fraction from MODIS satellite data, and the biomass burning preprocessor *Prep_chem_sources*, to calculate biomass burning emissions and grid anthropogenic emissions. Both a brief theoretical description of the preprocessors and technical instructions on how to install and run the preprocessor are given in the next two sections. The last section of this chapter explains how to run the Walter wetland model to generate CH_4 emissions from wetlands using the WRF meteorology to drive the model.

3.1 VPRM-Preprocessor

3.1.1 Description of the VPRM-Preprocessor

Two versions of the VPRM-Preprocessor are available, one producing output that can be used with WRF-GHG and one for the STILT-VPRM modeling system. Both versions are organized in two branches within the same SVN repository. The source code can be downloaded from http://www.bgc-jena.mpg.de/~rkretsch/vprmpreproc or contact rkretsch@bgc-jena.mpg.de to obtain the code.

The VPRM-Preprocessor was written in the R scripting language and runs under the Linux/Unix operation system. Some additional libraries and tools need to be installed before the VPRM preprocessor can be used.

- Subversion client (SVN) version control system
- R scripting language (obtained from http://cran.r-project.org)

- HDF5 tools (obtained from http://www.hdfgroup.org/HDF5)
- H4toH5 conversation tool (obtained from http://www.hdfgroup.org/h4toh5/)
- MODIS Land Data Operational Product Evaluation (LDOPE) tool (obtained from http://gcmd.nasa.gov/records/LDOPE.html)
- MODIS Reprojection Tool (MRT) (obtained from https://lpdaac.usgs.gov/lpdaac/tools/modis_reprojection_tool)
- NETCDF libraries and tools (obtained from http://www.unidata.ucar.edu/software/netcdf)

The VPRM-Preprocessor uses the Terra MODIS satellite level-3 land product (MOD 09A1 Surface Reflectance 8-Day L3, Global 500 m SIN Grid). The MODIS Surface Reflectance products provide an estimate of the surface spectral reflectance as it would be measured at ground level in the absence of atmospheric scattering or absorption. This MODIS-derived 8-day surface reflectance data product at 500 m resolution can be obtained as tile granules by using the web-service client WIST (Warehouse Inventory Search Tool) from the website http://wist.echo.nasa.gov after a free registration. The input data for the VPRM-Preprocessor are stored in the HDF-EOS (Hierachical Data Format Earth Observing System) file format. The MOD09A1 tiles for a given domain and yearly period are loaded into the VPRM-Preprocessor while running the program. Additionally, a pixel wise quality assessment and the EVI and LSWI calculation are performed with a data aggregation from 500 m resolution to 1 km resolution by a nearest–neighbor resampling process.

3.1.2 Installation, Configuration and usage of the VPRM-Preprocessor

After copying the VPRM-Preprocessor source code from the subversion repository, the following steps are needed to install and run the preprocessor:

1. Extracting the source code from the archive
2. Patching of the LDOPE tools
   Some modifications to `math_sds.c` and `cp_proj_param.c` are necessary. Patch files are included in the distribution of this preprocessor and can be found in the root directory of the preprocessor (`<PATH_TO_PREPROCESSOR>`) as the files `cp_proj_param.patch` and `math_sds.patch`. The patches have to be applied and afterwards the LDOPE tools have to be recompiled. Patches and recompiled LDOPE binaries can also be downloaded from http://www.bgc-jena.mpg.de/~rkretsch/vprmpreproc.
3. Configuration of the preprocessor by editing the `config.r` file

4. Preparation of the SYNMAP vegetation map
   Vegetation information is obtained from the SYNMAP by Jung et al. [2006] provided for the whole globe at 1 km horizontal resolution. Smaller domain areas (Europe, North America) are available from http://www.bgc-jena.mpg.de/~rkretsch/vprmpreproc. A SYNMAP file of one's own can be created by executing the shell script `get_synmap.sh` from `<PATH_TO_PREPROCESSOR>`. This shell script uses the `gridEurope.r` file from `<PATH_TO_PREPROCESSOR>/RSources` and can be configured for each domain.

After installation of the VPRM-Preprocessor, the main directory structure (`<PATH_TO_PREPROCESSOR>`) consists of the following subdirectories and files:

`<RSources>`	
`EVI.sh`	
`LSWI.sh`	
`get_synmap.sh`	
`preprocess.sh`	
`submit_loess.sh`	
`clean.sh`	
`clean_all.sh`	
`manual.odt`	short description in open office format
`apply_mapping.c`	
`check_output.sh`	
`apply_mapping_synmap.c`	
`submit_regrid.sh`	
`lsf_getmapping.r`	
`lsf_regrid.r`	
`check_output.r`	
`compile.sh`	
`tiles.txt`	will be created in VPRM preprocessor runs
`cp_proj_param.patch`	patched LDOPE tool
`math_sds.patch`	patched LDOPE tool
`submit_preproc.sh`	shell script for starting the VPRM-Preprocessor
`VPRMpreproc.r`	main program of the VPRM-Preprocessor
`config.r`	configuration file of the VPRM-Preprocessor
`process_loess.r`	
`lsf_run.log`	log file of the VPRM-Preprocessor run
`manual.pdf`	short description of the VPRM-Preprocessor

The R-script `VPRMpreproc.r` is the main program of the VPRM-Preprocessor and is executed by using the `submit_preproc.sh` shell script. The final output of the VPRM-Preprocessor is written as NetCDF files in the output directory, which can be set in the `config.r` file. All the configuration that is needed to run the VPRM-Preprocessor can

be done by editing the configuration file `config.r` file in the VPRM-Preprocessor path (`<PATH_TO_PREPROCESSOR>`). The following options can be set in the `config.r` file:

`mpath`	Working directory, must have write permission
`rdatain`	Path where input R data files are stored (SYNMAP vegetation map is located here)
`rdataout`	Path where intermediate R data files will be saved
`outdir`	Path where the final preprocessor output files are stored in NetCDF format
`modisrep`	Path where the MOD09A1 HDF-EOS tiles are stored
`modis_ver`	Version of the MOD09A1 land product - currently 005
`mrt`	Path where the MODIS Reprojection Tool (MRT) is stored
`ldope`	Path where MODIS Land Data Operational Product Evaluation (LDOPE) tool is saved
`domainname`	Name of your domain, which also affects the naming of the output subdirectory
`year`	Year to process
`synmaptouse`	Name of the SYNMAP vegetation map file. (You may create a SYNMAP file which covers your domain using `<PATH_TO_PREPROCESSOR>/Rsources/gridEurope.r)`
`do_parallel`	Logical flag which supports parallel preprocessing
`indices`	R vector of data types to be preprocessed (normally “evi” and “lswi”)
`nests`	Number of nests in your WRF-GHG run
`wrfinp`	Path to the WRF input files for obtaining the definition of domain and grid

The variables in the `config.r` configuration file specifying the domain settings (`ll.lon`, `ll.lat`,`nx`,`ny`,`dxx`,`dxy`) are obtained from the `wrfinput` file.

After the preprocessing has finished, the final output files will be stored in the defined output directory in the following seven NetCDF-files, which contain yearly data:

1. VPRM_input_VEF_FRA_yyyy.nc
2. VPRM_input_EVI_yyyy.nc
3. VPRM_input_EVI_MIN_yyyy.nc
4. VPRM_input_EVI_MAX_yyyy.nc
5. VPRM_input_LSWI_yyyy.nc
6. VPRM_input_LSWI_MIN_yyyy.nc
7. VPRM_input_LSWI_MAX_yyyy.nc

3.2 Biomass burning preprocessor: Prep_chem_sources

An explanation of the basic theoretical principles of the biomass burning preprocessor to calculate the biomass burning emissions is given in Sec. 2.3.2. Here, the description focuses more on the structure behind this preprocessor. A more technical description of this preprocessor can be found in Appendix B of the WRF-Chem user guide [Peckham et al., 2009].

3.2.1 Description of the preprocessor

This preprocessor was originally built for the Coupled Chemistry, Aerosol and Tracer Transport model to the Brazilian developments on the Regional Atmospheric Modeling System (CCATT-BRAMS) [Longo et al., 2007, Freitas et al., 2009] run at the Instituto Nacional de Pesquisas Espaciais (INPE) in Brazil and is now part of the WRF-Chem model when using the chemistry options 301 and 5 [Peckham et al., 2009]. In general, this preprocessor calculates biomass burning emissions derived from satellite fire spots for various species in [kg/m^2 day] on almost any user-defined grid. Additionally, necessary output for running the plumerise module (firesize, etc.) inside the WRF-GHG or the WRF-Chem model is provided. Furthermore, the preprocessor can be used for regridding of anthropogenic (EDGAR, RETRO, GOCART), biogenic and biomass burning (GFEDV2) emissions. The original code was obtained from National Institute for Space Research (INPE) in São José dos Campos, Brazil and augmented for NetCDF output. The routines dealing with the EDGAR emission database were also upgraded to be able to handle the EDGARV4.1 emission inventory. In general, the units of the output fields are [kg/m^2 day]. In case of using diurnal cycle routines, the units are [kg/m^2 s].

3.2.2 Running the preprocessor

A manual explaining how to run the *Prep_chem_sources* preprocessor is found in the WRF-Chem user guide Appendix B [Peckham et al., 2009]. Here, the main purpose is to describe how to run the preprocessor in order to obtain biomass burning emissions for CO_2, CH_4 and CO and EDGAR gridded output fields containing a diurnal cycle for the fossil fuel emissions. The code can be obtained on request via email to karla.longo@dge.inpe.br and saulo.freitas@cptec.inpe.br.

Compilation of the preprocessor

Before compiling in the preprocessor by typing the make command in the directory, one must ensure that all `*.mod` and `*.o` files as well as `prep_chem_sources.a` are deleted and that the correct compiler option is set in `include_prep_chem_src.mk`. If you have problems you can contact Thomas Koch (tkoch@bgc-jena.mpg.de). For very spe-

cific and detailed questions regarding the code of the biomass burning preprocessor contact the developers of the code, Karla Longo (karla.longo@dge.inpe.br) and Saulo Freitas (saulo.freitas@cptec.inpe.br).

Edit the `prep_chem_sources.inp` file

The "namelist" file of the preprocessor is called `prep_chem_sources.inp` and it is found in the `/bin` directory. The items described below are the main settings for producing WRF-GHG compatible output. The WRF grid projection has to be selected and the details regarding the projection that were set, e.g. in the WPS namelist, also have to be set here. It is recommended to not calculate the emissions for several nests in one single run, but rather run the preprocessor separately for each grid. Emission datasets that should not be used by the preprocessor will be noted with a 0 in the namelist.

Variable	**Value**	**Description**
gridtype of grid output		
`grid_type`	`polar`	polar projection used in WRF
	`lambert`	lcc projection used in WRF
	`gg`	gaussian grid projection
	`polar`	lat/lon projection
date of emission		
`ihour`	`0`	will be set in `work.sh` file
`iday`	`14`	will be set in `work.sh` file
`imon`	`7`	will be set in `work.sh` file
`iyear`	`2008`	will be set in `work.sh` file
selection of source dataset		
`use_edgar`	`1`	EDGAR emissions used
`use_bbm`	`1`	produce biomass burning emissions
`use_bbem_plumerise`	`1`	output for plumerise module in WRF
directories to be set		
`bbem_wfabba_data_dir`	`/...`	directory of WF_ABBA satellite data
`bbem_modis_data_dir`	`/...`	directory of modis satellite data
`bbem_inpe_data_dir`	`/...`	directory of INPE satellite data
`veg_type_data_dir`	`/...`	directory of vegetation type data
`carbon_density_data_dir`	`/...`	directory of carbon density data
regional grids		
`NGRIDS`	`1`	number of grids (keep it to 1)
`NNXP`	`200,`	number of x grid points
`NNYP`	`220,`	number of y grid points
`DELTAX`	`30000.`	X grid spacing in [m]
`DELTAY`	`30000.`	Y grid spacing in [m]
`POLELAT`	`45.`	For polar projection
`POLELON`	`-115.`	For polar projection
`STDLAT1`	`45.`	For lcc projection

STDLAT2	35.	For lcc projection
CENTLAT	45.	For lcc projection
CENTLON	-115.	For lcc projection

Run the preprocessor

To run the preprocessor, a shell script has been written (`work.sh`) that allows the preprocessor to be run either for many days (e.g. two months) or for one single day with hourly timestep to obtain a diurnal cycle for anthropogenic emissions. The runtime variables (`ihour`, `iday`, `imon`, `iyear`) are specified in the `work.sh` file. For a single day run (e.g. for calculating the diurnal cycle of the EDGAR emissions) `ihour` is set from 0 to 25. If biomass burning emissions are produced, `ihour` is kept constant and `iday` varies from 1 to 31 for a specific month. The following input variables for WRF-GHG are stored in NetCDF format: biomass burning emissions of CO_2, CH_4 and CO, plumerise module output for these species and EDGAR emissions for CO_2, CH_4 and CO. Furthermore, GRADs and binary output is produced for all species needed for the WRF-Chem chemistry options 5 and 301 (for more detail see Peckham et al. [2009]).

Main routines relevant for WRF-GHG

Here is a short description of the routines most relevant to the production of WRF-GHG input:

- `prep_chem_sources.f90`
  Main routine of the preprocessor. The subroutine calls for all emission datasets to be read in and gridded and the calls for the calculation of the biomass burning emissions are located here. Netcdf output was included in this routine for the biomass burning and EDGAR emissions and the plumerise module (marked with "(TK)"). In this routine the diurnal cycle for the EDGAR emissions can be turned off by uncommenting the subroutine call `diurnal_cycle_edgar`.

- `3bem_emissions.f90`
  Routine where the biomass burning emissions are calculated.

- `3bem_plumerise.f90`
  Routine to calculate the output for the plumerise module.

- `edgar_emissions.f90`
  Here changes have been made for an upgrade to version 4.1 of the EDGAR emission inventory (marked with either "(TK)" or "(VB)"). In particular, the prefix of the name of the EDGAR data files has to be specified in that routine. The extrapolation of the fossil fuel emissions with vehicle data for South America (`extrapoly_update`) can be turned off here.

3.3 Walter wetland model

A relatively short description of the different steps that are needed to calculate CH_4 wetland fluxes using the Walter wetland model driven by WRF meteorological output fields is given here. The code of the Walter wetland model was adapted to `fortran90` and partially restructured (*there is room for improvement in the future*). The theoretical background the Walter wetland model has already been described in Sec. 2.3.2. The order in which the single programs need to be run is described in the following (all fortran programs are easily compiled using e.g. the command `pgf90 -o a.out program.f90` if not specified otherwise) for the pgi fortran compiler:

1. Meteorological output from WRF
   Meteorological variables of the WRF netcdf output file have to be extracted at each wetland grid point as hourly values. The following variables are extracted from the WRF output field and written in `*.txt` format that is can be read by the Walter model: TSLB (`pTDs.dat, pTD3s.dat, PTD4s.dat, PTD5s.dat`), T2 (`temperature2.dat`), XLONG (`trans.matrix`), XLAT (`trans.matrix`), SWDOWN (`swdown2.dat`), WET
   MAP (`tot_frin_new.dat`), GLW (`glw2.dat`), RAINC (`tot_precip.dat`), RAINNC (`tot_precip.dat`), IVGTYP (`DATAin_tot.dat`), ISLTYP (`DATAin_tot.dat`) and TSK (`pTDs.dat, pTD3s.dat, PTD4s.dat, PTD5s.dat`). The program `wrfout_d02_May_09.f90` is used for this extraction and calculation.

2. Static fields
   All the static fields which were originally available on a $1.0° \times 1.0°$ grid for all wetland points of the global wetland map of Matthews and Fung [1987] have to be gridded to the WRF projection and missing values need to be filled in. This has to be done only once as these are static non-changing fields. In case of using a new wetland map, everything described under this point has to be re-preprocessed.

   - From the WRF model grid the latitudes and longitude values of each wetland grid point and the percentage of wetland coverage for each grid cell need to be extracted (the programm `wrfout_data_matrix_d02.f90` is used for that). This information will be stored in the `trans.matrix` file - which later will be used to retransform the wetland emissions calculated for each wetland grid point to a two-dimensional field - and in the `tot_frin_new.dat` file. The `DATAin_tot.dat` file contains the information about the values of the parameters described in Table 2.7 for each grid point that depends on the WRF vegetation and soil type.
   - Three external fields (mean annual soil temperature, annual NPP and the Laplace operator of the elevation) have to be gridded from the $1.0° \times 1.0°$ wetland points to the WRF wetland points. This is done by several small R programs (`regrid_dtmean.r`, `regrid_elevation.r`, `regrid_npp.r`). For the elevation a constant value of 750 is filled in for the missing values, the mean

annual soil temperature is set to a constant value of 27° e.g. for the Amazon region, while it has a latitudinal gradient for other regions of the globe for missing values. For the NPP, missing values were replaced by a mean NPP e.g. for the Amazon region while for other regions latitudinal gradients were applied. In case the R output is not fortran compatible, the programm `r_to_fortran.f90` can be run to get the right output format. Another option would be to not use the external fields provided by the Walter wetland model, but use your own mean annual soil temperature, NPP and elevation fields.

- For the hydrological model two static output fields are required, specifying the total bucket volume at each grid point (`Sy_tot.in_wrf`) and the bucket volume up to each soil layer (`Sy_vol.in_wrf`) at each single grid point. These are produced by running the program `Sy_make.f90`.

3. Hydrological model
   The hydrological model calculating the position of the water table is divided into two fortran programs, one for the calculation of the demand of evapotranspiration (`demand_d02.f90`) and one for the calculation of the water table (`bucket_d02.f90`).

   - For the calculation of the demand of evapotranspiration (`demand_d02.f90`) the files `temperature2.dat`, `swdown2.dat`, `glw2.dat` and `trans.matrix` are necessary input files from which the demand is calculated using equations described in Walter et al. [2001a]. The output file is called `Demand.in_wrf` which serves as input for the second program of the hydrological model.
   - Input files for the calculation of the water table in the hydrological bucket model (`bucket_d02.f90`) are: `DATAin_tot.dat`, `trans.matrix`, `Demand.in_wrf`, `tot_precip.dat`, `Sy_tot.in_wrf`, `Sy_vol.in_wrf` and `Elevation_in.dat`. From these drivers, the position of the water table is calculated for each day of the runtime (`Water.data`) as described in Walter et al. [2001a].

4. CH_4 flux model
   The main routine for the calculation of the CH_4 wetland emissions is called `Gmain_d02.f90`. It consists of the main program `Gmain_d02.f90` and three additional modules: `module_scalc.f90` for the calculation of parameters that are constant in time but spatially varying, `module_smodel.f90` for the calculation of the CH_4 emissions and `module_soutput.f90` for writing the output files. The command for the compilation is the following:

   ```
   pgf90 -o a.out Gmain_d02.f90 module_scalc.f90 module_smodel.f90
   module_soutput.f90
   ```

   Input data are the soil temperature at four different layers (`pTDs.dat, pTD3s.dat, PTD4s.dat, PTD5s.dat`), mean annual soil temperature (`Dtmean_xx.dat`), daily NPP (`Dfnpp_Nov.dat`), the position of the water table from the hydrological model (`Water.data`) and soil and vegetation parameters (`DATAin_tot.dat`). The model has two time steps. The outer time step (`ntime`) is set to the number of days for

which the model is run, while the inner time step (`nday`) is set to 24, meaning that fluxes are calculated on an hourly time scale, but the final output time step of the fluxes is daily. The output file is called e.g. `flux_test_d02.out`.

5. Retransformation to WRF grid
   Finally, the CH_4 fluxes that were calculated separately for each grid point have to be retransformed to the WRF grid and multiplied with the fraction of wetland coverage per grid cell. Therefore, `tot_frin_new.dat` and `flux_test_d02.out` serve as input files for the program `back_to_grid_d02.f90` which gives the NetCDF output of the calculated CH_4 fluxes.

Chapter 4

How to run WRF-GHG

This chapter is written to guide experienced WRF users through the new technical features of WRF-GHG. First, the different steps necessary to successfully run WRF-GHG are pointed out. The second section deals with namelist options, both the newly introduced ones for WRF-GHG and specific settings required for the WRF-GHG in the conventional WRF namelist options. In the last section the matlab script to fill of the arrays in the `wrfinput` file is described.

4.1 Steps to run WRF-GHG

As already mentioned above, this guide is written for WRF/WRF-Chem users with experience. Therefore, not each single step that is required to run the WRF model without the GHG model is explained in detail. To get started with WRF, it is recommend to work through the WRF online tutorial and have already done some WRF meteorology runs, before starting with WRF-GHG.

1. WRF-GHG is compiled in the same way as the usual WRF-Chem code. Set the path of your NetCDF library (and hdf library if it is required to build the NetCDF library), type `export WRF_CHEM=1` (using bash) to include the chemistry part in the compilation and then type `./configure` to choose your machine option (for mpi-bgc cluster users: type "4" for the machine and "1" for the nest option - for the WRF preprocessing system (not explained here) use "5" for the machine option). After that, compile the real data cases (`./compile em_real >& compile.log`) and make sure that all executables have been created.

2. All necessary preprocessed files (meteorology, trace gas fluxes, additional input fields) should be available in the right format, i.e. on the WRF grid.

3. Edit the `namelist.input` file. Specific settings regarding WRF-GHG are explained

in the next section.

4. Run `./real.exe` and check if all necessary tracer arrays that had been defined in the `registry.ghg` file are created as empty arrays in the `wrfinput` and `wrfbdy` files.

5. Run the compiled matlab script `co2_input_d01` (for mpi-bgc cluster users: to compile a matlab script type e.g. `mcc -m co2_input_d01`), e.g. with the command `sh run_co2_input_d01.sh /usr/local/apps/matlab/2010a` depending on your matlab version and the compiler settings, and check afterwards if the empty arrays in the `wrfinput` and the `wrfbdy` files are filled with reasonable values of the corresponding fields.

6. Run `./wrf.exe`
   (For submitting the `./wrf.exe` job on the MPI-BGC cluster, the shell script `start_wrf_pg8.sh` can be used with the command `sh start_wrf_pg8.sh 32` where 32 denotes the number of CPUs used.)

If the `wrfoutput` file is too big, the output can be reduced by excluding variables from the output in the `registry.ghg` file by deleting the "h" in the 8th column. In case of severe runtime problems that seem to have their origin in the GHG part, please contact the authors of this report.
To perform WRF-GHG simulations with daily re-initialization in an automatic way, the Model Organizing Software System (MOSS) is used at MPI-BGC. A description of how to use MOSS is given in Appendix C.

4.2 Namelist settings

In the `namelist.input` file settings are modified and the different possibilities for emissions and fluxes can be chosen for a WRF-GHG simulation. The `namelist.input` file has an augmentation in the `&physics` part of the original `namelist.input` file of the WRF-Chem model.
But the following chemistry options in the `namelist.input` file should be set as followed to allow for reasonable GHG tracer transport:

Variable	**Value**	**Description**
`chem_opt`	`98`	defines `GHG_TRACER` package and allows for GHG tracer transport
`vertmix_onoff`	`1`	to allow for vertical mixing of the tracer
`have_bcs_chem`	`.true.`	uses the right scheme to fill in the boundary conditions
`chem_in_opt`	`0`	no external emissions for WRF-Chem allowed
`emiss_inpt_opt`	`0`	no external emissions for WRF-Chem allowed
`chem_conv_tr`	`1`	to allow for subgrid convective tracer transport

The `&physics` section of the `namelist.input` file is augmented by the following options for tracer transport in WRF-GHG:

Variable	**Value**	**Description**
`vprm_class`	`8`	How many VPRM classes/vegetation types are used
`vprm_par_file`		`‘‘VPRM_param_CERES2005.txt"` Name of VPRM parameter file located in `<run/CO2_input>`
`co2_st_time`	`360`	Starting time for tracer transport in min if very high values (>10000) are assigned no tracer transport will take place
`co2_anthro`	`0`	no anthropogenic emissions
	`1`	daily anthropogenic emissions for CO_2, CH_4 and CO (external dataset)
	`2`	hourly anthropogenic emissions for CO_2, CH_4 and CO (external dataset)
`wetland_type`	`0`	no CH_4 wetland emissions
	`1`	floodplain and peatland CH_4 wetland emissions (Kaplan)
	`2`	only floodplain CH_4 wetland emissions (Kaplan)
	`3`	only peatland CH_4 wetland emissions (Kaplan)
	`4`	external CH_4 wetland emissions (Walter)
`file_term`		`‘‘CH4_termite_NW.txt"` `*.txt` file containing table of biomass and corresponding termite emissions for America and Australia (NW) `‘‘CH4_termite_OW.txt"` for Europe, Africa and Asia (OW) located in `<run/CH4_input>`
`term_id`	`0`	no termite emissions
	`1`	only CH_4 termite emissions
	`2`	CH_4 and CO_2 termite emissions
	`3`	only CO_2 termite emissions
	`4`	external CH_4 termite emissions
`bb_opt_ghg`	`0`	no biomass burning emissions
	`2`	biomass burning emissions (CO_2, CH_4 and CO) with plumerise module and diurnal cycle
	`3`	biomass burning emissions without plumerise module and diurnal cycle
	`4`	biomass burning emissions without plumerise module but with diurnal cycle
`plume_frq_ghg`	`180`	plumerise fire frequency in minutes (180 min recommended)
`soil_id`	`0`	no calculation of soil uptake fluxes

	1	calculation of soil uptake fluxes
	2	external soil uptake dataset
veg_id	0	no calculation of CH_4 emissions from vegetation
	1	calculation of CH_4 emissions from vegetation
	2	external CH_4 emissions from vegetation
oce_id	0	no CO_2 ocean fluxes
	1	external CO_2 ocean fluxes (hourly time step)

4.3 Matlab script

The matlab script `f_initialize_Amazon_d01.m` reads the `wrfinput` and `wrfbdy` file and fills in values for the initial and boundary conditions of the tracers as described in Sec. 2.2 and additionally reads in external data for the empty arrays defined in the `registry.ghg` file and created during compilation. For initial and boundary conditions a three-dimensional interpolation to the WRF grid is performed online. The different functions inside the Matlab script are briefly described in the following:

1. Functions to fill in initial conditions for CO_2, CH_4 and CO are called `f_CO2_TM3_IC`, `f_CH4_TM5_IC` and `f_CO_MACC_IC`. The initial conditions are usually filled in for the tracers that transport total CO_2, CH_4 and CO concentrations (*CO2_1*, *CH4_1* and *COT_1*) and for the background concentrations (*CO2_B*, *CH4_B* and *COT_B*). As already mentioned in Sec. 2.2 due to strong gradients in the concentrations for some regions on the globe (e.g. the Amazon) it is advisable to initialize all tracers (at least for tropical regions) either with the initial conditions or with a constant offset to avoid oscillation with negative values in the advection scheme which is the reason for "disappearing" fluxes.

2. Functions to fill in the lateral boundary conditions for CO_2, CH_4 and CO are `f_CO2_TM3_LBCs`, `f_CH4_TM5_LBCs` and `f_CO_MACC_LBCs`. All tracers that are initialized (as mentioned above) must have their boundary conditions set. If a coarse domain and a nested domain are used, the nested domain is only initialized, but gets its lateral boundary conditions from the coarse domain.

3. Function to read in the VPRM preprocessed fields (`f_vprm_in`) such as *VEG_FRA*, *EVI_MAX*, *EVI_MIN*, *LSWI_MAX* and *LSWI_MIN*.

4. As an example for anthropogenic emissions, hourly emissions from the EDGAR emission inventory are read with the function `f_edgar_in` into the WRF flux variables *FL_ANTCO2*, *FL_ANTCH4* and *FL_ANTCO*.

5. For the wetland emission either the function `f_wet_in` can be used to read in external wetland emissions as e.g. from the Walter model into the WRF flux variable *FL_WET* or the function `f_wet_kaplan_in` is used to read in the LPJ carbon pool

and the Kaplan potential wetland map (*CPOOL* and *WETMAP*) necessary for the online calculation of the CH_4 wetland fluxes using the Kaplan model.

6. The biomass burning emissions and plumerise variables are read in with the function `f_bbm_in`. Here the units of the biomass burning emissions have to be converted from [kg/m^2 day] to the flux units inside the WRF-GHG [kg/m^2 s]. The biomass burning emissions are linked to the following flux variables *FL_BBCO2*, *FL_BBCH4* and *FL_BBCO*. The fields of the plumerise module are linked to the following variables: *MEAN_FCT_AGTF_1*, *MEAN_FCT_AGEF_1*, *MEAN_FCT_AGSV_1*, *MEAN_FCT_AGGR_1*, *FIRESIZE_AGTF_1*, *FIRESIZE_AGEF_1*, *FIRESIZE_AGSV_1*, and *FIRESIZE_AGGR_1*.

7. To replace the ECMWF soil moisture with the GPNR soil moisture, the function `f_sm_in` is used. As this function is very short and easily comprehensible, it could serve as an example to write your own function for filling in your own dataset.

Appendix A

Coupling the GHG model to a new WRF release

The GHG model is coupled to the WRF-Chem model besides some minor modifications of the WRF-Chem code to allow for tracer transport and turning off several chemistry options by adding three modules in the `<chem>` directory and a new file to the `<Registry>` directory. In this chapter a detailed description of the routines that have been changed is given, such that the steps for an upgrade the WRF-GHG to a newer WRF-Chem version are traceable. All changes that have been made to the code are noted either with "RAR", "VB" or "VB-RAR" in the code. In this chapter the locations where the code has been changed are noted, but not all changes of the code are illustrated explicitly in this chapter.

`<chem>` directory

1. Copy the following files from the `<chem>` folder of the current WRF-GHG version into the `<chem>` folder of the new WRF-GHG version:
   - `module_greenhouse_gases.F`
   - `module_add_emissions.F`
   - `module_plumerise_ghg.F`
2. `/chem/Makefile`
   The three new modules have to be included in the `Makefile` of the chemistry part, so that the `*.f90` and `*.o` files can be created during the compilation of the code. In the current `Makefile` they are inserted in line 12 (`module_greenhouse_gases.o`), line 14 (`module_plumerise_ghg.o`) and line 18 (`module_add_emissions.o`).
   Also the dependencies of the modules from each other and from other modules have to be written into the `Makefile`:

`module_greenhouse_gases.o: module_add_emissions.o module_plumerise_ghg.o` (line 163)

`module_plumerise_ghg.o: module_zero_plumegen_coms.o module_chem_plumerise:scalar.o` (line 157)

`module_add_emissions.o:` (line 161)

`chem_driver.o: ... module_greenhouse_gases.o ...` (line 271)
to include the dependency of the `module_greenhouse_gases.o` from the `chem_driver.o` on other modules.

3. `/chem/chem_driver.F`

   - Insert the following line at the beginning of the `chem_driver.F` routine (line 44):
     `USE module_greenhouse_gases`
     to allow for the subroutine call `greenhouse_gases` in the `module_greenhouse_gases.F` from the `chem_driver.F`.
   - Implement call of the subroutine `greenhouse_gases` in the `chem_driver.F` (line 683-725) for `chem_opt == 98`.
   - A WRF debug call was implemented (line 425) for the `GHG_TRACER` package
   - The calculation of aerosol properties (line 826), photolysis rate (line 848) and other chemical mechanisms (line 1028) are turned off for the mode of tracer transport, as only vertical mixing and dry deposition (optional) are used as chemistry mechanisms for tracer transport, by inserting the line

     `config_flags%chem_opt / = GHG_TRACER`

4. `/chem/module_input_chem_data.F`
   To set the determintation of the last gas species of the GHG_TRACER package to zero by adding the lines (line 2835):

   ```
   case (GHG_TRACER)
   get_last_gas = 0
   ```

   There might be some other comments (without any effect) in that routine.

5. `/chem/chemics_init.F`
   Exclusion of chemistry initialization (no initialization of standard profiles) (line 283):

   `IF(config_flags%chem_opt == 98) RETURN`

   Additionally, a short text notice about the WRF-GHG model is written in here.

6. /chem/module_vertmx_wrf.F
   Since WRF version V3.2 all changes that had been made in previous versions in that routine have already been included into the official WRF-Chem release.

7. /chem/dry_dep_driver.F
   The Wesely dry deposition mechanism is excluded by adding the line

   config_flags%chem_opt / = GHG_TRACER (line 176)

   There are some additional notes without changes in the code in that routine.

<Registry> directory

1. /Registry/registry.ghg
   Copy that file from the current WRF-GHG version to the <Registry> folder of the new WRF-GHG version.

2. /Registry/Registry.EM_CHEM
   Add the following line into the Registry.EM_CHEM file to include the registry .ghg in the actual registry that is used for building the code (line 444):
   include registry.ghg

3. Registry/registry.dimspec
   In this file, all the dimensions used in the WRF model are defined. For the VPRM parameters, the number of simulation hours and namelist parameters of additional variables have to be defined in the following way (lines 75-77):

```
dimspec   0  2  namelist=vprm_class     z  VPRM_vegetation_classes
dimspec   1  2  namelist=run_hours      z  Simulations_hours
dimspec   1  2  namelist=wetland_type   z  wetland_type
```

<run> directory

Create the folders <CO2_input> and <CH4_input> in the <run> directory and copy the *.txt files from both folders of the current WRF-GHG model version to the newly established folders. These files contain the information about the parameters of the VPRM model and the emission fluxes per unit biomass for the termite emissions.

<dyn_em> directory

1. /dyn_em/module_initialize_real.F
   Here the calls of the subroutines used to read in the *.txt files containing the VPRM

parameter and termite emission parameters are located:

`CALL VPRM_par_initialize` (line 2020)
`CALL termite_initialize` (line 2026)

2. `/dyn_em/solve_em.F`
In that routine it is determined that the tracer transport starts after a certain time that is specified with the value of the variable `co2_st_time` in the `namelist.input` file (line 2142).
`BENCH_START(chem_adv_tim)`
`chem_scalar_advance: IF (num_3d_c >= PARAM_FIRST_ SCALAR .AND. config_flags%co2_st_time < grid%xtime) THEN`

3. `/dyn_em/start_em.F`
Here the call of the subroutine `chem_init` is prohibited if the greenhouse gas tracer package is used (line 1031):
`IF ( config_flags%chem_opt /=98 )THEN`

<share> directory

1. `/share/mediation_integrate.F`
If the `GHG_TRACER` package is used WRF-Chem will be prevented from reading in auxiliary chemical input variables by adding the following line to the code:

`IF( config_flags%chem_opt > 0 .AND. config_flags%chem_opt / = 98 ) THEN` (line 86)

2. `/share/solve_interface.F`
Here again the time control for tracer transport and emissions is implemented:
`IF(config_flags%chem_opt == 98 .AND. config_flags%co2_st_time<grid %xtime ) THEN`

3. `/share/module_model_constants.F`
Two subroutines to read in the `*.txt` files for the VPRM parameters and the termite emission parameters are located in that routine (line 161, 197):

`SUBROUTINE VPRM_par_initialize`
`SUBROUTINE termite_initialize`

<main> directory

The chemistry initialization for the nest will be prohibited by inserting the following code to these `/main/ndown_em.F` (line 692, 729), `/main/real_em.F` (line 445, 511) and

`/main/nup_em.F` (line 636,655) routines:

```
IF(parent_grid%chem_opt .NE. 0 .AND. parent_grid%chem_opt /= 98)
then
```

And also a message is written out in these routines:

```
ELSE
message = 'RAVAN: NO INITIALIZATION for CO2_* in this step'
CALL wrf_message (message) (line 729)
```

Appendix B

Figures

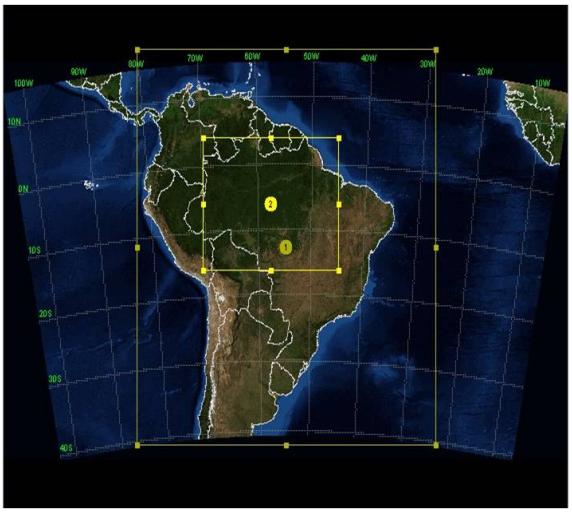


Figure B.1: Sketch of an example for a model domain (here the Amazon region) for WRF-GHG simulations illustrating a coarse (30 km, "d01") and a nested model domain (10 km, "d02").

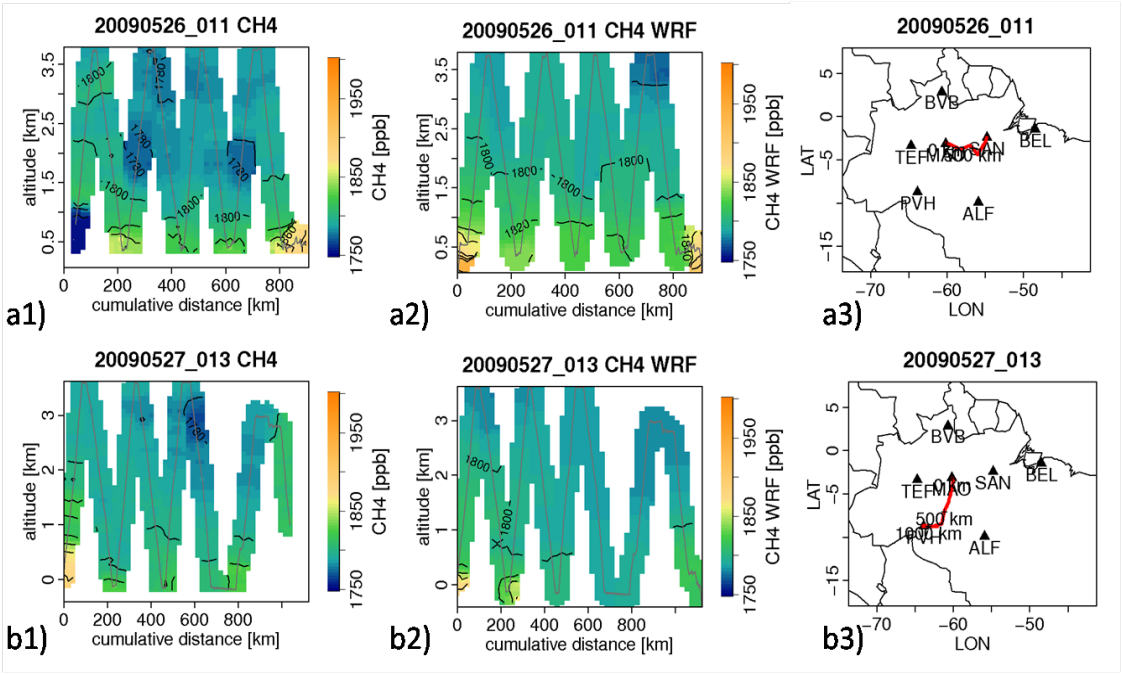


Figure B.2: Comparison of observed CH_4 mixing ratios (a1,b1) to the WRF simulated CH_4 concentrations (a2,b2) in vertical cross-sections along the flight path (a3,b3) of the airplane for two flights in the Amazon region during the BARCA project. The grey lines denotes the vertical "path" of the airplane flown, where the mixing ratios have been measured. The observations are interpolated in the same way as the WRF-GHG results which had been extracted along the flight path of the airplane. CH_4 concentration is indicated by the color scale.

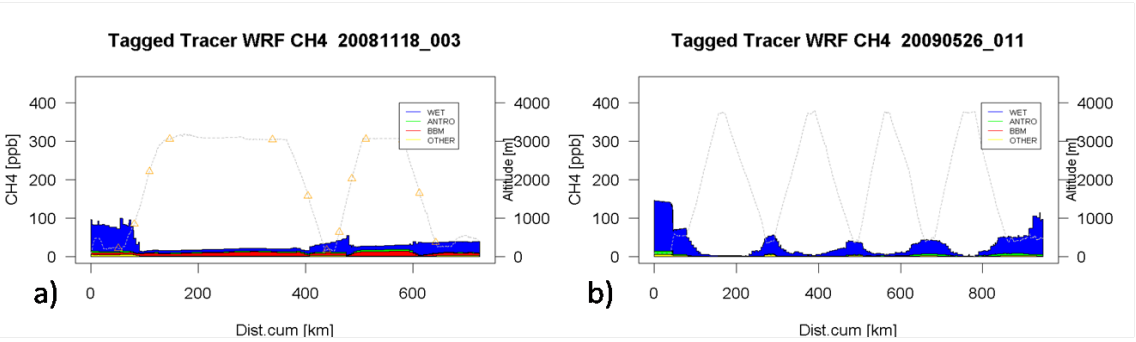


Figure B.3: Extracted tagged tracer for different CH_4 emission processes along the flight path for two flights in the Amazon during the BARCA project. The sum of all components is the difference of the total CH_4 concentration ($CH4\_1$) and the CH_4 background concentration ($CH4\_B$). (a) illustrates one flight at the end of the dry season in November 2008 with significant biomass burning contribution, while for (b) at the end of the wet season the CH_4 emissions from wetlands are dominating.

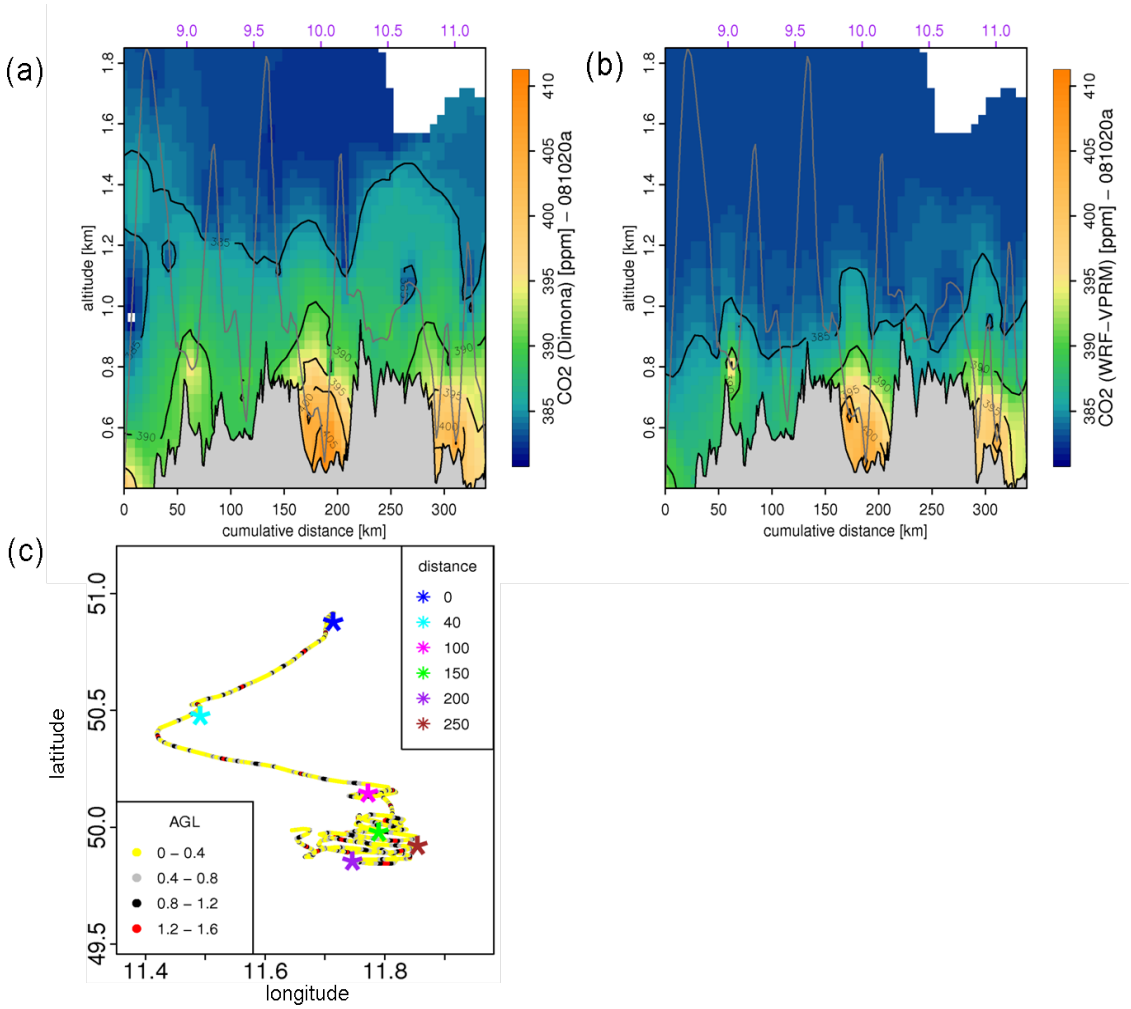


Figure B.4: Vertical cross section (using a distance weighted interpolation) of the observed and simulated CO_2 fields (given in ppm) as a function of distance flown by the aircraft (cumulative distance) around the Ochsenkopf Tower in Fichtelgebirge, Germany, for 20th October 2008: a) measurements b) WRF-VPRM simulations within the European domain c) Flight track with color gradient showing altitude range (legend at the top left-hand side of the panel) above ground. The symbol "*" denotes cumulative distance in km (legend at the bottom right-hand side of the panel). In (a-b), the time of measurements/simulations is given in the top X-axis.

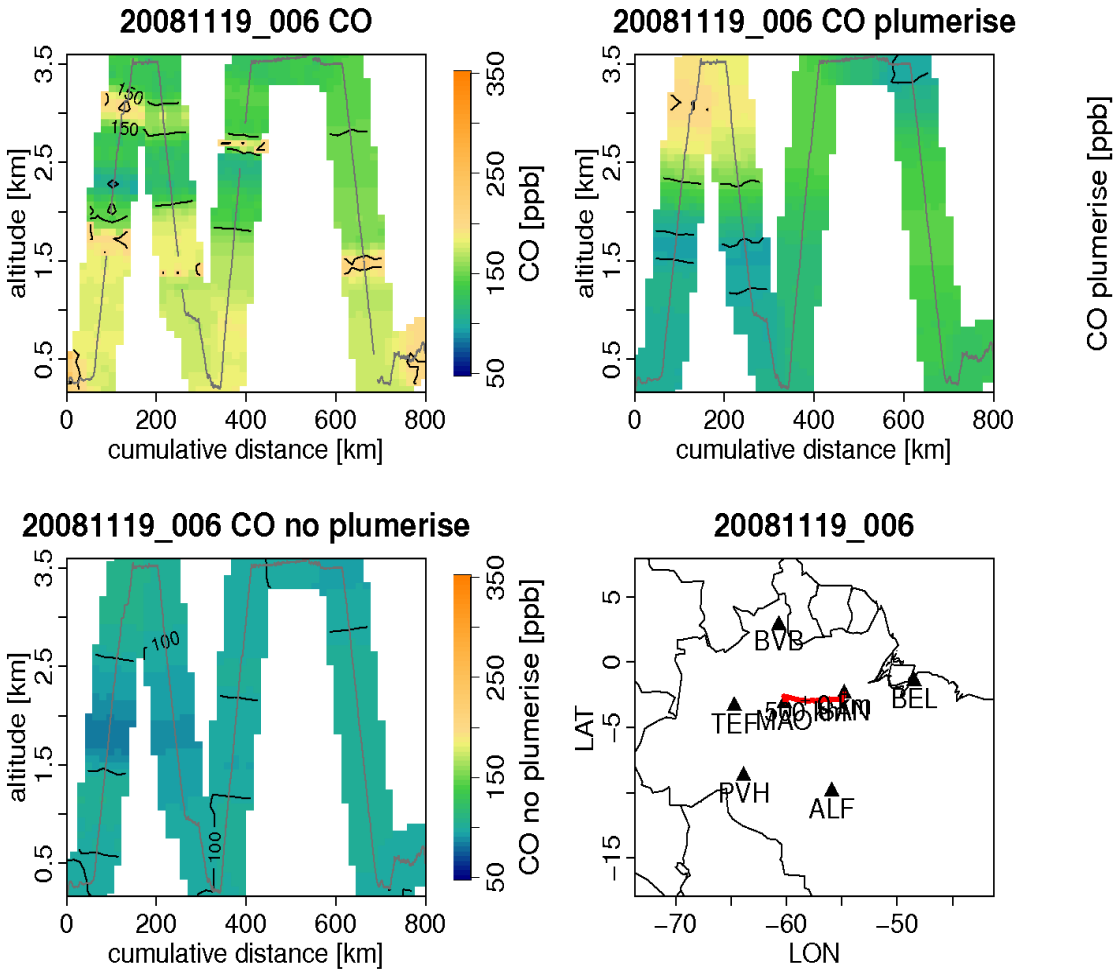


Figure B.5: Vertical cross section of observed CO concentrations along a flight track (a) on 19th November 2008 in the Amazon region from Santarém to Manaus compared to WRF-GHG simulations using the plumerise mechanism (b) and WRF-GHG simulations without using the plumerise mechanism (c).

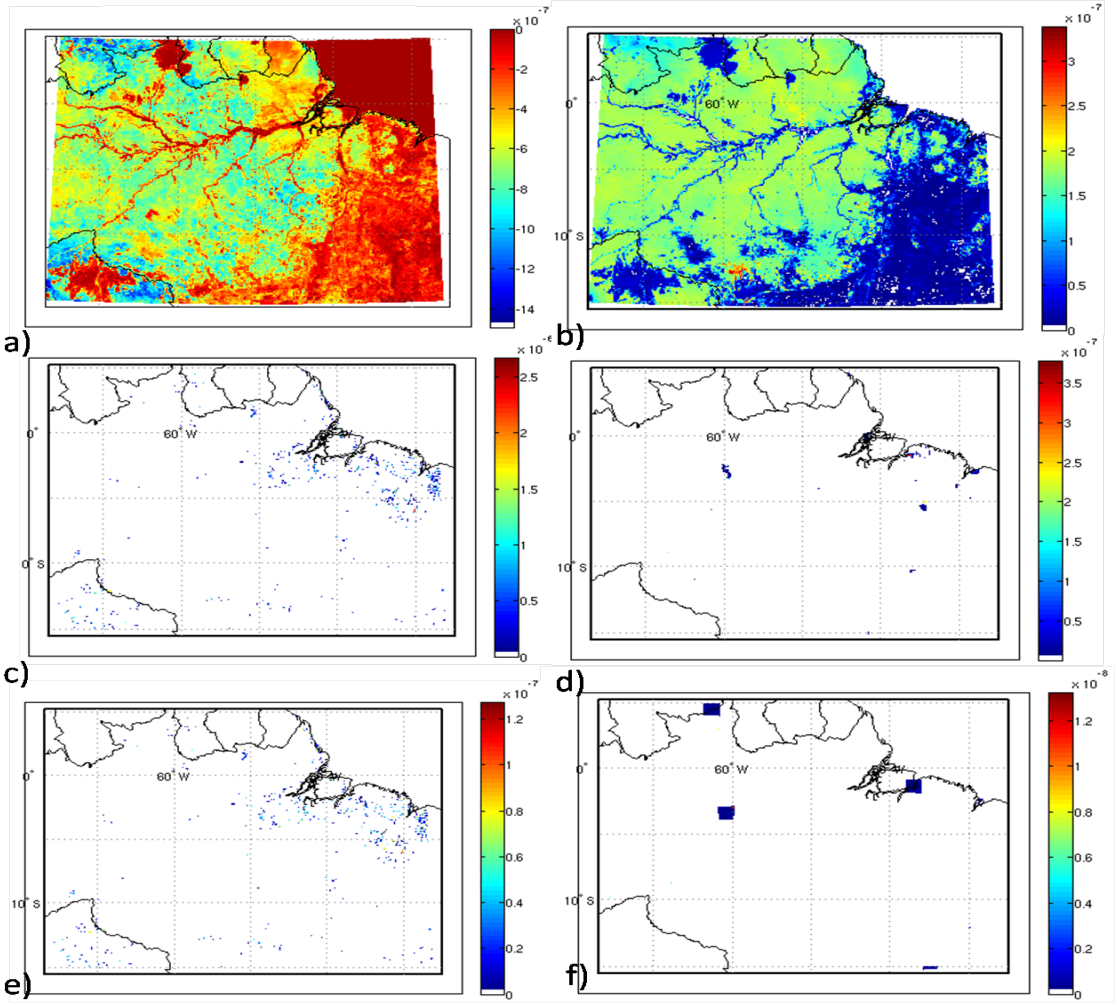


Figure B.6: Example for CO_2 and CO fluxes over the Amazon basin simulated by WRF-GHG. For that simulation, the VPRM model - calculating biospheric CO_2 fluxes GEE (a) and respiration (b), the biomass burning preprocessor for the calculation of CO_2 (c) and CO (e) biomass burning fluxes for 20th November 2008 and the EDGAR emission inventory for anthropogenic emissions of CO_2 (d) and CO (f) were utilized. All units are in [kg/m^{2}s].

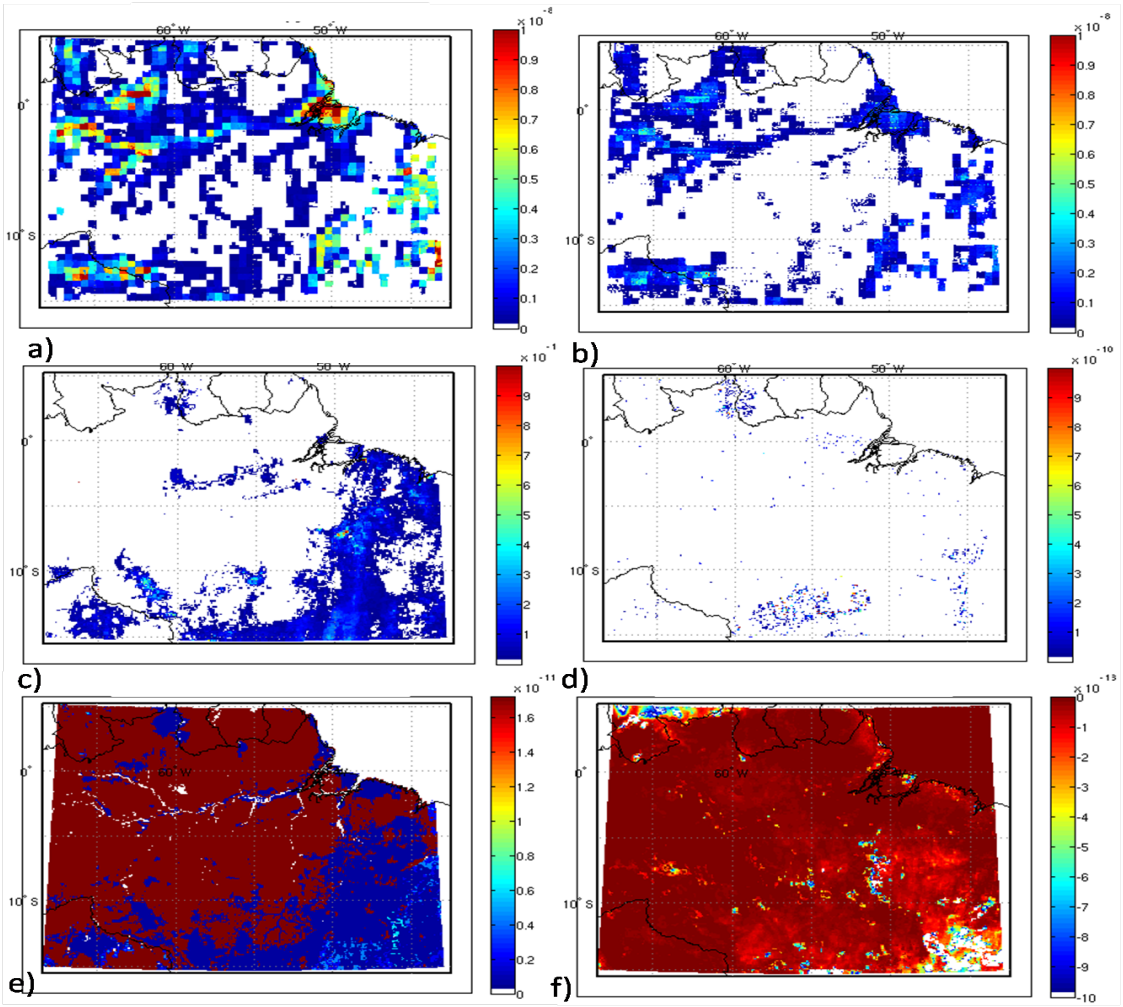


Figure B.7: Example for CH_4 fluxes over the Amazon basin, using the online calculated wetland fluxes of the Kaplan inventory (a) or the offline calculated wetland fluxes using the Walter model (b), anthropogenic emissions from the EDGAR emission inventory (c), biomass burning emissions from the biomass burning preprocessor for 20th November 2008 (d), online calculated termite emissions (e) and soil uptake of CH_4 from the atmosphere (f). All units are in [kg/m^{2}s].

Appendix C

Model Organizing Software System (MOSS)

The Model Organizing Software System (MOSS) has been developed by Roberto Kretschmer (rkretsch@bgc-jena.mpg.de) to automatize and organize WRF-VPRM (now WRF-GHG) model simulations that allow for daily re-initialization of meteorology. It is written in Python language and automates the daily start of the 30 hr WRF simulation for each day, taking the tracer fields from the previous day as initialization (see Sec. 2.2). MOSS submits WRF runs to the Institute's computing cluster using the load sharing facility (LSF). Output generated by WRF is automatically saved in a central archive that is managed by the software. In addition, MOSS uses a data base management system (MySQL database of the Institute) to persistently store meta-information for all the runs performed and the files that were created. This makes it easy to find runs and the associated model output by querying the database using any of user interfaces (UI). Currently there are three UIs available to access MOSS: 1) web browser interface (described in Kretschmer [2008]) 2) Python graphical user interface (GUI, shown here) 3) the standard MySQL command line interface. A backup of the meta-information and the actual data is performed regularly on the Institutes tape archives maintained by the IT department to prevent data loss. A detailed description of the MOSS is found in Kretschmer [2008]. Here the focus is on a short introduction to use the MOSS to perform WRF-GHG simulations.

C.1 Steps to start a WRF-GHG simulation with MOSS

Basically, the MOSS executes the steps 4-6 described in Sec. 4.1 automatically for each short-term forecast of the simulation period. A separate module can be defined for each new user specifying the name of the matlab script (Sec. 4.3), the number of domains for which the matlab script has to be executed, and which files should be stored (e.g.

`wrfinput`,`wrfbdy`, `wrfoutput`, `namelist.input`, etc.). To start a WRF-GHG simulation with MOSS, the following steps are required:

```
 &time_control
 run_days                            = 0,
 run_hours                           = 30,
 run_minutes                         = 0,
 run_seconds                         = 0,
 start_year                          = {start_year}, {start_year}, {start_year},
 start_month                         = {start_month},   {start_month},   {start_month},
 start_day                           = {start_day},   {start_day},   {start_day},
 start_hour                          = 18,   18,   12,
 start_minute                        = 00,   00,   00,
 start_second                        = 00,   00,   00,
 end_year                            = {end_year}, {end_year}, {end_year},
 end_month                           = {end_month},   {end_month},   {end_month},
 end_day                             = {end_day},   {end_day},   {end_day},
 end_hour                            = 00,   00,   12,
 end_minute                          = 00,   00,   00,
 end_second                          = 00,   00,   00,
 interval_seconds                    = 21600
 input_from_file                     = .true.,.true.,.true.,
 history_interval                    = 180,  60,   60,
 history_begin_h                     = 06,  06,   00,
 frames_per_outfile                  = 1000, 1000, 1000,
 restart                             = .false.,
 restart_interval                    = 5000,
 io_form_history                     = 2
 io_form_restart                     = 2
 io_form_input                       = 2
 io_form_boundary                    = 2
 debug_level                         = 0
 io_form_auxhist2                    = 2
 /

 &domains
 time_step                           = 180,
 time_step_fract_num                 = 0,
"namelist.input.template" 219L, 8672C
```

Figure C.1: Part of the `namlist.input.template` file showing the changes necessary to be done in the `time_control` section to allow for the handing over of the MOSS date variables `End date` and `Start date`.

1. Before starting MOSS, the matlab scripts (cf. Sec. 4.3) have to be compiled by using e.g. the command `mcc -m co2_input_d01.m` and the `run_co2_input_d01.sh` file should be created in the Matlab directory.

2. The `namelist.input` file has to be modified as illustrated in Fig. C.1 to allow the handing over of the different dates and the tracer restart defined in the run setting of MOSS. The modified file is saved as `namelist.input.template` (might be located in the `<WRFV3>` directory) and the path to the file is set up in the run settings (6.).

3. Create a `<wrf-result>` directory (e.g. in the `<WRFV3/run>` directory). In this directory MOSS creates links to the WRF history files (`wrfoutput`) of each previous short-term forecast in order to perform the restart of tracer fields for a consistent transport simulation.

4. Start MOSS by executing `moss.sh` in the directory `</Net/Groups/BSY/tools/MOSS>`. The MOSS GUI is loaded and presents the user a dialogue window as illustrated in Fig. C.2. To configure simulations and access data two menu entries can be found in the main menu: `Run` and `Module`.

5. Under the button `Module` and `Select`, a specific module can be selected to start the

WRF-GHG simulations (e.g. as example `mod_barca` (see Fig. C.4) for a simulation with one nest or `mod_rkretsch` for a simulation with only one domain)

6. A new MOSS run (needed to be setup for each new WRF-GHG simulation) is defined by selecting the option `Run` → `New` in the MOSS GUI (Fig. C.2). A new dialogue (see Fig. C.3) asks the user to setup the run specification. The run specifications should be set in the following way:

`Name`	Defining name of the WRF-GHG simulation
`Description`	(optional) to specify changes/specific settings
`Start date`	First day of the WRF-GHG simulation
`End date`	Last day of the WRF-GHG simulation
`WRF path`	Path to the `wrf.exe` executable
`Namelist path`	Path to the `namelist.input.template` file
`WRF result path`	Path to the `<wrf-result>` directory
`Matlab path`	Path to the compiled matlab files
`Number of CPU's`	(optional) Set number of CPU used for the simulation (standard 24)
`Queue`	(optional) To change the queue on the Cluster

7. The WRF-GHG simulation is started by selecting the menu entry `Run` → `Start`

8. For each job submitted from MOSS to the queue, the user receives an Email that contains status information of the cluster job (e.g. processors used, wall clock time, error messages).

9. Output files specified to be saved can be accessed by selecting `Run` → `Browse` files. In a dialogue window the user can query the data base to search for certain files and create links to these files in the archive in any directory the user desires. The archive location of the output files is in the directory `</Net/Groups/BSY/data/MOSS/run_ID>`. This directory contains subdirectories for each MOSS module that were used by the run.

Under certain circumstances (server failure, script abortion) MOSS might not quit correctly which hinders the normal operation. In such cases it is in general sufficient to delete the file `MOSS_update.lock` that is located in the user's home directory. After doing so the run has to be started again using the MOSS GUI.

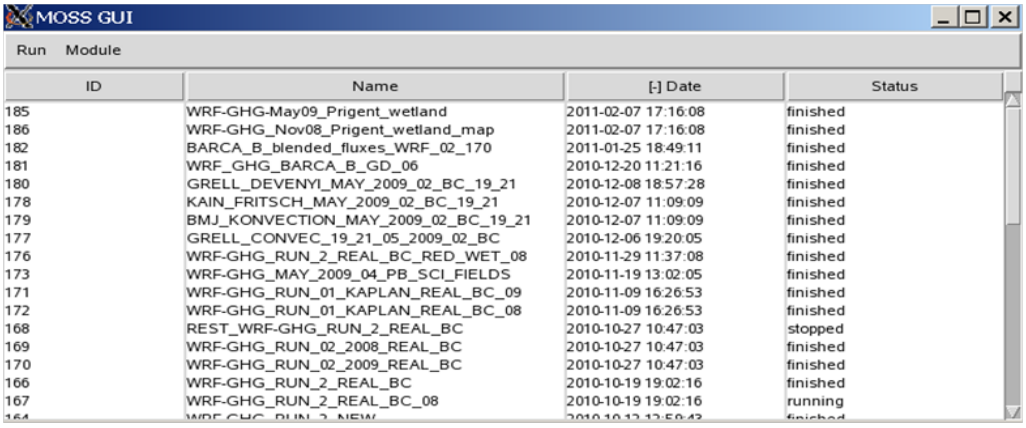


Figure C.2: MOSS GUI showing the ID of the run, the name of the run, the date when the run was started and the status of the run is shown and two buttons to select options for run and module settings.

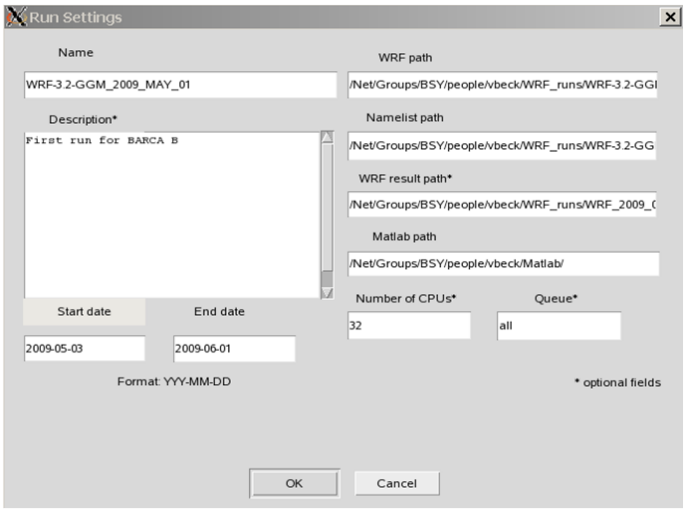


Figure C.3: Illustration of the window where the settings for a specific WRF-GHG simulation have to be specified.

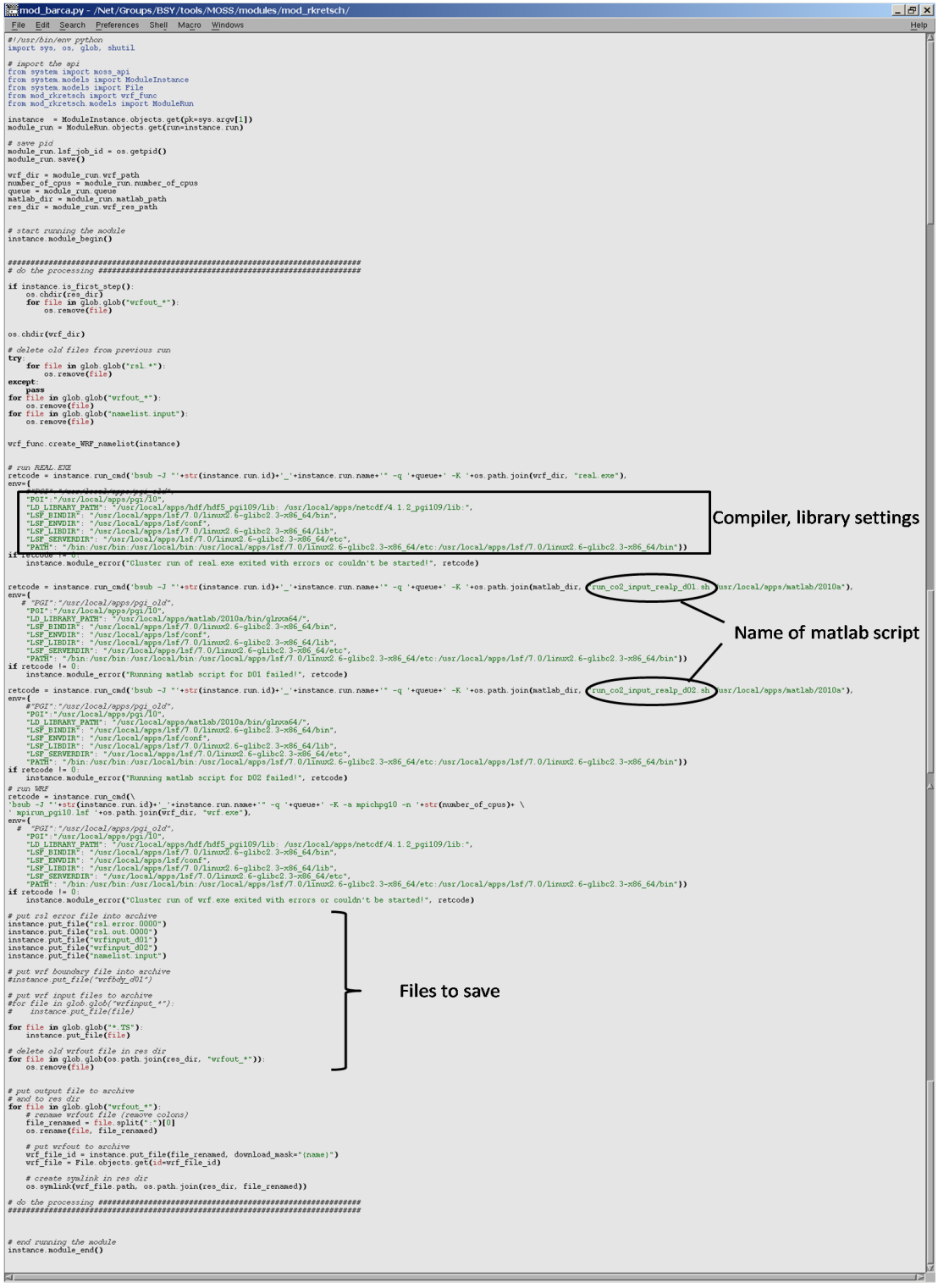

mod_barca.py - /Net/Groups/BSY/tools/MOSS/modules/mod_rkretsch/
File Edit Search Preferences Shell Macro Windows Help
Compiler, library settings
Name of matlab script
Files to save

Figure C.4: Example of a MOSS module file where compiler and library settings, name of the matlab scripts, submission commands for jobs to the cluster and the number of files to store are set.

Appendix D

Running WRF-GHG without Matlab

In case one should want to run WRF-GHG on a computer on which Matlab is not available, such as on blizzard, the supercomputer of the DKRZ (Deutsches Klimarechenzentrum), the task of filling in the flux fields and the initial and boundary conditions in the `wrfinput` and `wrfbdy` files (all of the tasks outlined in Sec. 4.3) can be done by using the command line netCDF operators of NCO. Information, source code, and documentation regarding NCO are available at `http://nco.sourceforge.net/`.

NCO comprises twelve different stand-alone commands that use netCDF files as input, perform a range of operations, and write netCDF files as output. By carefully combining these commands and preparing the pre-processed flux fields and boundary condition concentration fields as netCDF files (with any required interpolation already completed), the entire Matlab program can be replaced by a shell script. All examples given in this appendix are written using bash syntax.

More complete documentation can be found in the NCO User's Guide, but a brief introduction to the operators, describing only their functionality as they are used in the script, is given here.

`ncks` (netCDF Kitchen Sink): Extracts subsets of data (specified variables and attributes plus all global data) from an input file and writes it in netCDF format to an output file. This is the most-used of all the operators in the script.

`ncecat` (netCDF Ensemble Concatenator): Combines an arbitrary number of netCDF input files into a single netCDF output file, storing each of the input files as a single record in the output file. This is useful when WRF expects hourly fluxes, but the input data are constant in time, as it allows for the same variable to be easily repeated for each record.

`ncbo` (netCDF Binary Operator): Performs binary operations on variables stored in two input files, and saves the results in an output file. This was used in the script for the calculation of the tracer lateral boundary conditions, in order to calculate the tendencies (*BTYS*, *BTXE*, etc.) by subtracting the boundary values at adjacent time steps. Furthermore, these tendencies need to be divided by the number of seconds in 6 hours (21600 s, the time step in the boundary condition files). To do this a netCDF file was created with a variable containing a constant value (1/21600) on the model's grid, and `ncbo` was used to multiply the two variables together.

`ncpdq` (netCDF Permute Dimensions Quickly): Rearranges the order of dimensions for given variables, getting them into the order required by WRF.

`ncrcat` (netCDF Record Concatenator): Concatenates record variables across an arbitrary number of files.

`ncrename` (netCDF Renamer): Renames dimensions, variables, and attributes in a netCDF file.

`ncflint` (netCDF File Interpolater): Makes a linear combination of different input files either as a weighted average (as is used in an example below), a normalized weighted average, or an interpolation.

As an example of how a simple, time-invariant field is put into the `wrfinput` file, consider the case of the Kaplan potential wetland map and the LPJ carbon pool (WETMAP and CPOOL), both of which are required for online calculation of methane wetland fluxes based on the Kaplan model. In Sec. 4.3 this is described in item 5, and carried out with the Matlab function `f_wet_kaplan_in`. Using NCO this can be done as follows (shown only for WETMAP, CPOOL is equivalent):

```
wrfin=${workdir}'/wrfinput_d0'${d}
```

Here the `wrfinput` file is being defined, where `d` specifies the number of the domain, and acts as the index in a for-loop for simulations with multiple domains. The working directory has been previously defined in the script.

```
wetfile=${inputdir}'/new_wetlands_d0'${d}'.nc'
```

The original potential wetland map has already been interpolated to the grid resolution of the domain offline.

```
ncks -v Wetlands $wetfile dummy.nc
```

Here `ncks` is used to extract just the variable of interest, "`Wetlands`", and saves it in a temporary file called `dummy.nc`.

```
ncecat dummy.nc dummy2.nc
```

The concatenation operator `ncecat` is used here not to concatenate files but rather to add a record dimension (which will be renamed to "`Time`") to the variable such that it matches the dimensionality of the `wrfinput` file.

```
ncrename -v Wetlands,WETMAP -d ncl0,south_north -d ncl1,west_east \
   -d record,Time dummy2.nc
```

`ncrename` is used to replace both the variable and all the dimension names in order to match the `wrfinput` file.

```
ncks -A  -v WETMAP dummy2.nc $wrfin
rm dummy*
```

Finally, the *WETMAP* variable is written into the `wrfinput` file and all the intermediary working files are removed.

For the VPRM pre-processed fields roughly the same procedure can be followed for the following variables: *VEG_FRA*, *EVI_MAX*, *EVI_MIN*, *LSWI_MAX*, and *LSWI_MIN*. However for variables *EVI* and *LSWI* it's a bit more complicated as the day of the year needs to be taken into account, and a weighted average taken between adjacent values 8 days apart. When using Matlab, this would be carried out by `f_vprm_in` as described by item 3 in Sec. 4.3. Here is how it was done using NCO and shell scripting:

```
fld=( evi lswi )
fld_upper=( EVI LSWI )
```

This just saves the original variable names (`fld`) and the target variable names (`fld_upper`) as arrays that can be looped over.

```
for (( m=0; m<= 1; m++ ))
  do
  file_vprm=${vprmdir}/VPRM_input_${fld_upper[m]}_d0${d}_${year}.nc
  doy_string=$(ncks -d start_day_of_year $file_vprm)
  start_doy=${doy_string: -30:3}
  let "diff=$doy-$start_doy-2"
```

Here the day of the year, (`doy`), has already been calculated earlier in the script based on the month and day, while the initial day of the year in the VPRM input file (`file_vprm`) is extracted from the file using `ncks` and then subsampling the string. The difference between the two is calculated, and two is subtracted to account for zero indexing.

```
  let "n1=$diff/8"
  let "n0=$n1-1"
  let "n2=$diff%8"
  w1=$(echo "scale=3; 1-$n2/8.0" | bc)
  w2=$(echo "scale=3; 1-$w1" | bc)
```

Here the record numbers of the two adjacent 8-day time steps are calculated (`n0` and `n1`), and the weighting assigned to each of them. In order to average the two time steps using this weighting, each is first stored its own dummy file using `ncks`, and then `ncflint` is used to linearly average with the given weights:

```
  ncks -A  -d time,$n0 -v ${fld[m]} $file_vprm dummy1.nc
  ncks -A  -d time,$n1 -v ${fld[m]} $file_vprm dummy2.nc
  ncflint -v ${fld[m]} -w $w1,$w2 dummy1.nc dummy2.nc dummy3.nc
```

Now the file `dummy3.nc` has the required information, but the dimensions are in the wrong order, and have to be shuffled with `ncpdq`, renamed using `ncrename`, and inserted into `wrfinput` using `ncks`:

```
  ncpdq -v ${fld[m]} -a time,vprm_classes,south_north,west_east dummy3.nc dummy4.nc
  ncrename -v ${fld[m]},${fld_upper[m]} -d time,Time dummy4.nc
  ncks -A  -v ${fld_upper[m]} dummy4.nc $wrfin
  rm dummy*
done
```

Between these two examples and the comments on the operators themselves, the reader should have sufficient information to construct a script of his or her own to initialize the `wrfinput` and `wrfbdy` files based on specific model set-up and input data. One general recommendation would be to choose a grid with a different number of grid boxes along the lateral grid axes, which ensures that the correct data cannot be inserted into the target file transposed.

The script which initialized the `wrfinput` and `wrfbdy` files (`initialize_bdy.bash`) is run from another shell script (`runner.bash`) which, in order, copies the just-completed results to the output directory, updates the namelist automatically for the next day's simulation (using `sed` and dates extracted from the previous run's `wrfout` files), submits

`real.exe` to the queue, runs `initialize_bdy.bash`, and then submits `wrf.exe` to the queue. While lacking most of the functions of the MOSS, it allows for the automated production of the job string and re-initialization of the input files without any interactive input. Both of these scripts were developed by Julia Marshall (marshall@bgc-jena.mpg.de) in order to run WRF-GHG on blizzard, and she should be contacted in case of any questions.

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